(12) INTERNATIONAL APPLICATION PUBLISHED UNDER THE PATENT COOPERATION TREATY (PCT)

CORRECTED VERSION

EXPRESS MAIL NO. EV934845916US

(19) World Intellectual Property Organization
International Bureau

(43) International Publication Date
24 October 2002 (24.10.2002)

PCT

(10) International Publication Number
WO 02/083854 A2

(51) International Patent Classification[7]: C12N

(21) International Application Number: PCT/US02/11521

(22) International Filing Date: 12 April 2002 (12.04.2002)

(25) Filing Language: English

(26) Publication Language: English

(30) Priority Data:
60/283,794 13 April 2001 (13.04.2001) US
60/303,689 6 July 2001 (06.07.2001) US

(71) Applicant *(for all designated States except US)*: **BIOGEN, INC.** [US/US]; 14 Cambridge Center, Cambridge, MA 02142 (US).

(72) Inventors; and
(75) Inventors/Applicants *(for US only)*: **LYNE, Paul,** D. [IE/US]; 72 Allston Street #3, Allston, MA 02139 (US). **GARBER, Ellen, A.** [US/US]; 14 Donnell Street, Cambridge, MA 02138 (US). **SALDANHA, Jose, W.** [GB/GB]; 21 Fillebrook Avenue, Enfield, Middlesex EN1 3BD (GB). **KARPUSAS, Michael** [US/GR]; Platonos 7, Agios Basilios, 26500 Patra (GR).

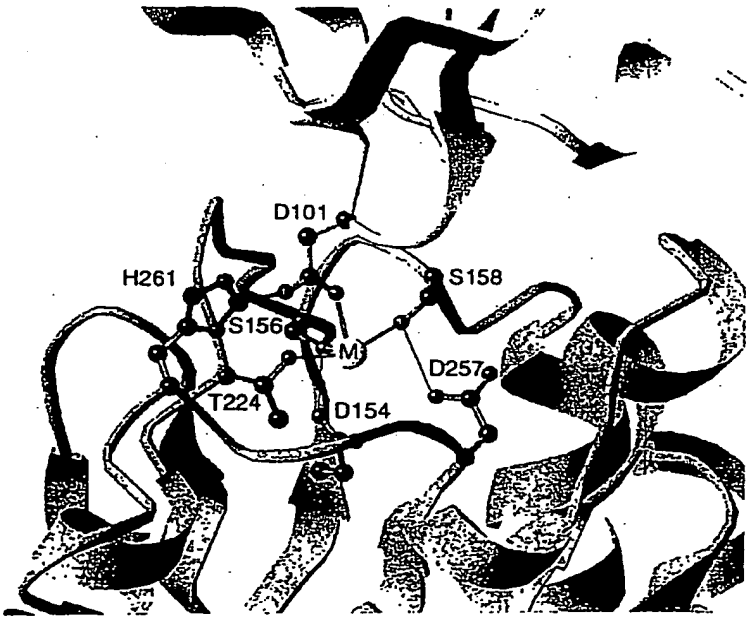
(74) Agents: **PIERRI, Margaret, A.** et al.; Fish & Neave, 1251 Avenue of the Americas, New York, NY 10020 (US).

(81) Designated States *(national)*: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW.

(84) Designated States *(regional)*: ARIPO patent (GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW),

*[Continued on next page]*

(54) Title: ANTIBODIES TO VLA-1




(57) Abstract: Antibodies that specifically bind to VLA-1 integrin and methods of using these antibodies to treat immunological disorders in a subject. Also included are crystal structures of complexes formed by VLA-1 antibodies and their ligands, and VLA-1 antagonists and agonists identified by using the structure coordinates of these structures.

WO 02/083854 A2

Eurasian patent (AM, AZ, BY, KG, KZ, MD, RU, TJ, TM), European patent (AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR), OAPI patent (BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG).

**Published:**

— *without international search report and to be republished upon receipt of that report*

**(48) Date of publication of this corrected version:**
6 November 2003

**(15) Information about Correction:**
see PCT Gazette No. 45/2003 of 6 November 2003, Section II

*For two-letter codes and other abbreviations, refer to the "Guidance Notes on Codes and Abbreviations" appearing at the beginning of each regular issue of the PCT Gazette.*

# ANTIBODIES TO VLA-1

## FIELD OF THE INVENTION

This invention relates to antibodies to VLA-1 integrin and the use of these antibodies in treating inflammatory diseases and other immunological disorders.

This invention also relates to the crystal structure of the complex between one such antibody and the α1-I domain of VLA-1, and to the use of this structural information for computational drug design.

## BACKGROUND OF THE INVENTION

Integrins are a superfamily of cell surface receptors that mediate cell-cell and cell-matrix adhesion. These proteins are known to provide anchorage as well as signals for cellular growth, migration and differentiation during development and tissue repair. They have been implicated in immune and inflammatory processes.

Integrins are heterodimeric proteins composed of two noncovalently linked polypeptide chains, α and β. The amino terminus of each chain forms a globular head that contributes to interchain linking and to ligand binding. The globular heads are connected to the transmembrane segments by stalks. The cytoplasmic tails are usually less than 50 amino acid residues long. Integrin subfamilies were originally defined on the basis of which β subunit was used to form the heterodimers. The β1-containing integrins are also called VLA molecules, referring to "very late activation" antigens. VLA-1 to VLA-6 refer to β1 subfamily members containing α1 to α6 (i.e., CD49a to CD49f), respectively. For general

review, see *Cellular and Molecular Immunology*, eds. Abul K. Abbas et al., W.B. Saunders Company, Philadelphia, PA, 2000.

Collagen (both types I and IV) and laminin are known ligands of α1β1 integrin (i.e., VLA-1). VLA-1 has been implicated in cell adhesion and migration on collagen (Keely et al., 1995, *J. Cell Sci.* 108:595-607; and Gotwals et al., 1996, *J. Clin. Invest.* 97:2469-2477); in promoting contraction and reorganization of collagen matrices, a critical component of wound healing (Gotwals et al., *supra*; and Chiro, 1991, *Cell* 67:403-410); and in regulating the expression of genes involved in extracellular matrix remodeling (Riikonen et al., 1995, *J. Biol. Chem.* 270:1-5; and Langholz et al., 1995, *J. Cell Biol.* 131:1903-1915). Thus, improper regulation of VLA-1 may result in certain pathological conditions such as fibrosis.

Moreover, it has been suggested that VLA-1 may play a role in T cell /monocyte-driven diseases. Anti-VLA-1 antibodies block T-cell dependent cytokine expression (Miyake et al., 1993, *J. Exp. Med.* 177:863-868). Expression of VLA-1 is increased in persistently activated, 2 to 4 week old cultured T cells (Hemler et al., 1985, *Eur. J. Immunol.* 15:502-508). VLA-1 is also expressed on a high percentage of T cells isolated from the synovium of patients with rheumatoid arthritis (Hemler et al., 1986, *J. Clin. Invest.* 78:692-702).

Several crystal structures of integrin α subunits have been determined, including the structures of the α2-I domain of α2β1 (PDB accession code 1aox; Emsley et al., 1997, *J. Biol. Chem.* 272:28512-28517); the α1-I domain of rat α1β1 (PDB accession number 1ck4; Nolte et al., 1999, *FEBS Lett.* 452:379-385; WO 00/20459); the α1 subunit of human α1β1 (PDB accession code 1qc5; Rich et al., 1999, *J. Biol. Chem.* 274:24906-24913); the αL-I and αM-I domains; and vWF-A3 (Lee et al., 1995, *Cell* 80:631-635; Lee et al., 1995, *Structure* 3:1333-1340; Qu et al., 1995, *Proc. Natl. Acad. Sci. USA* 92:10277-10281; Qu et al., 1996, *Structure* 4:931-942). The α2β1 structure revealed a helix (i.e., the C-helix) that created a trench or groove on one face of the protein at the metal-ion binding site (Emsley et al., *supra*). The crystal structure of the α2-I domain complexed to a short collagen-based triple helical peptide revealed that the collagen-based peptide was bound to that trench, where the α2-I amino acids that made intermolecular or metal contacts included

Asp151, Asn154, Tyr157, Gln215, Asp219, Leu220, Thr221, Asp254, Glu256, His258, Tyr285, Leu286, Asn289, Leu291, Asn295, and Lys298 (PDB accession code 1dzi; Emsley et al., 2000, *Cell* 101:47-56; WO 01/73444). The amino acid numbering immediately above is based on PDB accession code 1dzi and herein referred to as "crystal numbering." The crystal structures of the rat and human α1-I domains revealed a similar trench.

## SUMMARY OF THE INVENTION

The present invention provides anti-VLA-1 antibodies and methods of using these antibodies to treat a variety of inflammatory and immunological disorders.

Specifically, the invention embraces an antibody that specifically binds to VLA-1 (e.g., human VLA-1). This antibody contains light chain complementarity determining regions ("CDR"s) defined by amino acid residues 24 to 33, 49 to 55, and 88 to 96 of SEQ ID NO:1, and/or heavy chain complementarity determining regions defined by amino acid residues 31 to 35, 50 to 65, and 98 to 107 of SEQ ID NO:2. These CDRs may contain mutations (e.g., deletions, insertions and/or substitutions) in the non-antigen-contacting portions, as determined from the crystal structure disclosed herein, without affecting the VLA-1-binding activity of the antibody. Exemplary mutations are S24N, G92S and D101A in the light chain CDRs, and G55S in the heavy chain CDR2. In one embodiment, the antibody of this invention contains a light chain variable domain sequence of SEQ ID NO:1 and/or a heavy chain variable domain sequence of SEQ ID NO:2.

In a related embodiment, the antibody of this invention contains the same heavy and light chain polypeptide sequences as an antibody produced by hybridoma mAQC2, deposited on April 18, 2001 at the American Type Culture Collection ("ATCC"), 10801 University Boulevard, Manassas, VA 20110-2209 and having ATCC accession number PTA3273. (All ATCC deposits recited herein were made under the Budapest Treaty). This antibody can be produced by, for example, hybridoma mAQC2, or cells containing nucleic acid sequences isolated from that hybridoma that encode the heavy and light chains of the mAQC2 monoclonal antibody.

In another embodiment, the antibody is a humanized antibody comprising at least one (e.g., 2, 3, 4, or 5) of the following residues in its light chain: Q1, L4, P46, W47 and Y71; or at least one (e.g., 2, 3, 4, 5, 6 or 7) of the following residues in its heavy chain: D1, V12, S28, F29, A49, T93, R94 (Kabat numbering convention). For instance, the antibody comprises Q1, L4 and Y71 in the light chain; and/or (i) F29, A49, T93 and R94, or (ii) A49 and T93, in the heavy chain.

The humanized antibody of this invention may contain a light chain variable domain sequence defined by amino acid residues 1 to 106 of SEQ ID NO:3, and/or a heavy chain variable domain sequence defined by amino acid residues 1 to 118 of SEQ ID NO:4. The humanized antibody may comprise the same heavy and/or light chain polypeptide sequences as an antibody produced by cell line hAQC2 (ATCC accession number PTA3275; deposited on April 18, 2001).

In another embodiment, the humanized antibody of this invention may contain a mutation (e.g., deletion, substitution or addition) at one or more (e.g., 2, 3, 4, 5, 6, 7 or 8) of certain positions in the heavy chain such that an effector function of the antibody (e.g., the ability of the antibody to bind to a Fc receptor or a complement factor) is altered without affecting the antibody's ability to bind to VLA-1 (U.S. Patent 5,648,260). These heavy chain positions include, without limitation, residues 234, 235, 236, 237, 297, 318, 320 and 322 (EU numbering system). The humanized antibody can, for instance, contain the mutations L234A (i.e., replacing leucine at position 234 of an unmodified antibody with alanine) and L235A (EU numbering system) in its heavy chain. In one related embodiment, the antibody comprises the same heavy chain polypeptide sequence as an antibody produced by cell line hsAQC2 (ATCC accession number PTA3356; deposited on May 4, 2001).

In yet another embodiment, the humanized antibody of this invention may contain a mutation (e.g., deletion or substitution) at an amino acid residue that is a site for glycosylation, such that the glycosylation site is eliminated. Such an antibody may be clinically beneficial for having reduced effector functions or other undesired functions while retaining its VLA-1 binding affinity. Mutations of glycosylation sites can also be beneficial for process development (e.g., protein expression and purification). For instance, the heavy chain of the antibody may

contain the mutation N297Q (EU numbering system) such that the heavy chain can no longer be glycosylated at this site. In one related embodiment, the humanized antibody may comprise the same heavy chain polypeptide sequence as an antibody produced by cell line haAQC2 (ATCC accession number PTA3274; deposited on April 18, 2001).

In still other embodiments, the heavy and/or light chains of the antibody of this invention contain mutations that increase affinity for binding to VLA-1 and thereby increase potency for treating VLA-1-mediated disorders.

Embraced in this invention are also a composition containing an antibody of the invention and a pharmaceutically acceptable carrier; an isolated nucleic acid containing a coding sequence for SEQ ID NO:1; an isolated nucleic acid containing a coding sequence for SEQ ID NO:2; an isolated nucleic acid containing a coding sequence for the light chain of an antibody produced by hybridoma mAQC2; an isolated nucleic acid containing a coding sequence for the heavy chain of an antibody produced by hybridoma mAQC2; an isolated nucleic acid containing a coding sequence for the light chain of an antibody produced by cell line hAQC2; an isolated nucleic acid containing a coding sequence for the heavy chain of an antibody produced by cell line hAQC2; an isolated nucleic acid containing a coding sequence for the heavy chain of an antibody produced by cell line haAQC2; an isolated nucleic acid containing a coding sequence for the heavy chain of an antibody produced by cell line hsAQC2; an isolated nucleic acid containing a coding sequence for residues 1 to 106 of SEQ ID NO:3; an isolated nucleic acid containing a coding sequence for residues 1 to 118 of SEQ ID NO:4; cells of hybridoma mAQC2; cells from cell line hAQC2; cells from cell line haAQC2; and cells from cell line hsAQC2.

The present invention also provides a method of treating a subject with an immunological disorder mediated by VLA-1, including administering to the subject an effective amount of an antibody of this invention. For instance, this method is used to treat a human subject to palliate, ameliorate, stabilize, reverse, prevent, slow or delay progression of the disorder. Alternatively, this method is used prophylactically to treat a human subject at risk for developing this immunological disorder so as to

prevent or delay the onset of the disorder. An "effective amount" of the composition can be administered in one or more dosages.

VLA-1 mediated immunological disorders include, but are not limited to, disorders in which the VLA-1 activity level is elevated in one or more tissues as compared to a normal subject. Examples of such disorders are skin related conditions (e.g., psoriasis, eczema, burns, dermatitis, and abnormal proliferation of hair follicle cells), fibrosis (e.g., kidney or lung fibrosis), allergic rhinitis, respiratory distress syndrome, asthma, bronchitis, tendinitis, bursitis, fever, migraine headaches, gastrointestinal conditions (e.g., inflammatory bowel disease, Crohn's disease, gastritis, irritable bowel syndrome, colitis and colorectal cancer), vascular diseases (e.g., atherosclerosis), periarteritis nodosa, thyroiditis, aplastic anemia, Hodgkin's Disease, rheumatic fever, osteoarthritis, autoimmune diseases (e.g., type I diabetes, myasthenia gravis, rheumatoid arthritis, systemic lupus erythematosus, and multiple sclerosis), sarcoidosis, nephrotic syndrome, renal failure, Bechet's Syndrome, polymyositis, gingivitis, hypersensitivity (e.g., delayed type hypersentivity or immediate hypersensitivity), graft and transplant rejections, graft versus host disease (GVHD), conjunctivitis, swelling occurring after injury, myocardial ischemia, and endotoxin shock syndrome.

The present invention also provides a method of determining the level of VLA-1 in a tissue (e.g., tissue specimen and body fluid) comprising contacting the tissue (e.g., *in vivo* or *in vitro*) with the antibody of the invention, and then detecting the binding of the antibody to the tissue, thereby determining the level of VLA-1 in the tissue.

As used herein, the antibody of this invention can be, for instance, a murine antibody, a humanized antibody, or a chimeric antibody. It can be a whole antibody (i.e., with two full length light chains and two full length heavy chains) of any isotype and subtypes (e.g., IgM, IgD, $IgG_1$, $IgG_2$, $IgG_3$, $IgG_4$, IgE, $IgA_1$ and $IgA_2$; with either kappa or lambda light chain). Alternatively, the antibody of this invention refers to an antigen-binding fragment (e.g., Fab, $F(ab')_2$, and single chain Fv) of a whole antibody.

The present invention further provides crystallizable compositions and crystals of complexes formed by a rat-human chimeric α1-I domain (mutant RΔH) and a hAQC2 Fab fragment, and methods for using such compositions and crystals. This invention also provides the structure coordinates and binding sites of the chimeric domain and the hAQC2 Fab fragment. The atomic coordinates derived from the crystal structure described herein provide a structural basis for the biological activities of hAQC2 as well as a basis for rational design of VLA-1 agonists or antagonists with predicted biological activities (e.g., small molecule compounds or antibodies such as hAQC2 variants).

The crystal structure disclosed herein is the first crystal structure of an α1-I domain of an α1β1 integrin/ Fab complex. This structure shows the residues critical for Fab binding by α1-I domain. In addition, the Fab binds in the putative collagen-binding site and inhibits collagen binding. Amino acid residues found in the binding site on the α1-I domain include Asp154, Ser156, Asn157, Ser158, Tyr160, Glu192, Glu218, Arg219, Gly220, Gly221, Arg222, Gln223, Thr224, Asp257, His261, Asn263, Arg291, and Leu294 (crystal numbering). Residues on the Fab fragment found to bind to the α1-I domain include light chain residues Asn30, Tyr48, Trp90, Ser91, Asn93 and Trp95, and heavy chain residues Ser30, Arg31, Trp47, Ser52, Gly53, His56, Tyr58, Phe99, Gly100 and Asp101 (crystal numbering).

This invention also provides a computer for producing a three-dimensional representation of a molecular complex, where the molecular complex is defined by the set of structure coordinates of a complex of a chimeric I domain of an α1β1 integrin RΔH and humanized antibody hAQC2, according to Fig. 19; or a homologue of the molecular complex, the homologue having a root mean square deviation from the backbone atoms of the amino acids of not more than 0.65 Å. The computer includes a machine-readable data storage medium including a data storage material encoded with machine-readable data, where the data contains at least a portion of the structure coordinates of the complex according to Fig. 19; a working memory for storing instructions for processing the machine-readable data; a central-processing unit coupled to the working memory and to the machine-readable data storage medium for processing the machine readable data into the three-dimensional

representations; and a display coupled to the central-processing unit for displaying the three-dimensional representation.

This invention further provides a computer for producing a three-dimensional representation of a molecule or molecular complex including a binding site defined by structure coordinates of hAQC2 amino acids including at least seven (e.g., 7, 8, 9, 10, 11, 12, 13, 14, 15, or 16) of light chain residues Asn30, Tyr48, Trp90, Ser91, Asn93 and Trp95, and heavy chain residues Ser30, Arg31, Trp47, Ser52, Gly53, His56, Tyr58, Phe99, Gly100 and Asp101 (crystal numbering), according to Fig. 19; or a homologue of the molecule or molecular complex, where the homologue includes a binding site that has a root mean square deviation from the backbone atoms of the hAQC2 amino acids of not more than 1.10 Å. This invention also provides a computer for producing a three-dimensional representation of: a binding site defined by structure coordinates of hAQC2 amino acids including at least seven (e.g., 7, 8, 9, 10, 11, 12, 13, 14, 15, or 16) of light chain residues Asn30, Tyr48, Trp90, Ser91, Asn93 and Trp95, and heavy chain residues Ser30, Arg31, Trp47, Ser52, Gly53, His56, Tyr58, Phe99, Gly100 and Asp101 (crystal numbering), according to Fig. 19; a binding site of a homologue that has a root mean square deviation from the backbone atoms of the hAQC2 amino acids of not more than 1.10 Å.

This invention also provides a method for identifying an inhibitor of an I domain of an integrin including the steps of using structure coordinates of hAQC2 amino acids including at least seven (e.g., 7, 8, 9, 10, 11, 12, 13, 14, 15, or 16) of light chain residues Asn30, Tyr48, Trp90, Ser91, Asn93 and Trp95, and heavy chain residues Ser30, Arg31, Trp47, Ser52, Gly53, His56, Tyr58, Phe99, Gly100 and Asp101 (crystal numbering), according to Fig. 19 or ± a root mean square deviation from the backbone atoms of the hAQC2 amino acids not more than 1.10 Å, to generate a three-dimensional structure of a binding site; employing the three-dimensional structure to design or select a potential antagonist; synthesizing the potential antagonist; and contacting the potential antagonist with hAQC2 to determine the ability of the potential antagonist to interact with hAQC2, where the ability of the potential antagonist to interact with hAQC2 indicates that the potential antagonist is

an inhibitor of the I domain. This invention further provides an inhibitor of I domain of integrin identified by this method.

This invention also provides a computer for producing a three-dimensional representation of a molecule or molecular complex including: a binding site defined by structure coordinates of I domain amino acid residues Asp154, Ser156, Asn157, Ser158, Tyr160, Glu192, Gln218, Arg219, Gly220, Gly221, Arg222, Gln223, Thr224, Asp257, His261, Asn263, Arg291, and Leu294 (crystal numbering), according to Fig. 19; or a homologue of the molecule or molecular complex, where the homologue includes a second binding site that has a root mean square deviation from the backbone atoms of the I domain amino acids not more than 0.65 Å. This invention also provides a computer for producing a three-dimensional representation of: a first binding site defined by structure coordinates of I domain amino acids residues Asp154, Ser156, Asn157, Ser158, Tyr160, Glu192, Gln218, Arg219, Gly220, Gly221, Arg222, Gln223, Thr224, Asp257, His261, Asn263, Arg291, and Leu294 (crystal numbering), according to Fig. 19; or a binding site of a homologue that has a root mean square deviation from the backbone atoms of the I domain amino acids not more than 0.65 Å.

This invention also provides a computer for producing a three-dimensional representation of a molecule or molecular complex including: a binding site defined by structure coordinates of I domain amino acids including at least three of residues Glu192, Gln218, Arg219, Gly220, and Gly221 (crystal numbering), according to Fig. 19; or a homologue of the molecule or molecular complex, where the homologue includes a second binding site that has a root mean square deviation from the backbone atoms of the I domain amino acids not more than 1.0 Å. The invention further provides a computer for producing a three-dimensional representation of a binding site defined by structure coordinates of I domain amino acids including at least three of residues Glu192, Gln218, Arg219, Gly220, and Gly221 (crystal numbering), according to Fig. 19; or a binding site of a homologue that has a root mean square deviation from the backbone atoms of the I domain amino acids not more than 1.0 Å.

This invention further provides methods for using these three-dimensional representations to design chemical entities that associate with the chimeric domain or the hAQC2 Fab fragment, or portions thereof; and act as potential inhibitors of the chimeric domain or the hAQC2 Fab fragment, or portions thereof. This invention also relates to compositions including chemical entities, such as inhibitors and variants of the chimeric domain or variants of the hAQC2 Fab fragment, where such chemical entities and variants are rationally designed by means of the structure coordinates of the chimeric domain or the hAQC2 Fab fragment, or binding sites. The invention further relates to use of the above-identified chemical entities to treat or prevent conditions associated with inappropriate or abnormal $\alpha 1\beta 1$ activity in a subject.

This invention further provides a method for identifying an inhibitor of an I domain of an integrin including the steps of using the structure coordinates of I domain amino acids residues Asp154, Ser156, Asn157, Ser158, Tyr160, Glu192, Gln218, Arg219, Gly220, Gly221, Arg222, Gln223, Thr224, Asp257, His261, Asn263, Arg291, and Leu294 (crystal numbering), according to Fig. 19, to generate a three-dimensional structure of a binding site; employing the three-dimensional structure to design or select a potential antagonist; synthesizing the potential antagonist; and contacting the potential antagonist with I domain to determine the ability of the potential antagonist to interact with I domain, where the ability of the potential antagonist to interact with the I domain indicates that the potential antagonist is an inhibitor of the I domain.

This invention also provides a method for identifying an inhibitor of an I domain of an integrin including the steps of using the structure coordinates of at least three of I domain amino acids including residues Glu192, Gln218, Arg219, Gly220, and Gly221 (crystal numbering), according to Fig. 19, or ± a root mean square deviation from the backbone atoms of the I domain amino acids not more than 0.65 Å, to generate a three-dimensional structure of a binding site; employing the three-dimensional structure to design or select a potential antagonist; synthesizing the potential antagonist; and contacting the potential antagonist with I domain to determine the ability of the potential antagonist to interact with I domain of integrin,

where the ability of the potential antagonist to interact with the I domain indicates that the potential antagonist is an inhibitor of the I domain. This invention also provides an inhibitor of I domain of integrin identified by this method.

Other features and advantages of the invention will be apparent from the following detailed description, and from the claims.

## BRIEF DESCRIPTION OF THE DRAWINGS

**Figure 1.** *Collagen-binding integrins α1β1 and α2β1 on activated leukocytes.* (A). Flow cytometric analysis of α1 and α2β1 integrin expression on IL-2-activated splenocytes (d 11). Cells were labeled with either anti-α1 mAb, anti-α2 mAb, or non-binding control mAb (grey lines), and followed by FITC-anti-hamster immunoglobulin. (B) Effect of anti-α1 and anti-α2 mAbs on leukocyte adhesion to collagen. $10^5$ IL-2 activated splenocytes were treated with indicated mAbs for 15 min before plating onto either type IV or type I collagen-coated wells for 1 h at 37°C. Adhesion was calculated as illustrated in Example 1, and expressed as % adhesion relative to control mAb-treated cells. Adhesion assays were done in triplicate, and at least three independent experiments were performed. One representative experiment is shown.

**Figure 2.** *Effect of anti-integrin mAbs on the effector phase of delayed-type hypersensitivity.* SRBC-sensitized mice were injected i.p. with the indicated mAbs 1 h prior to SRBC challenge. Footpad thickness was measured 20 h after antigen challenge, and results shown as % increase in footpad thickness ± SEM as illustrated in Example 2. These data represent a summary of eight experiments with n = 79 (PBS), 68 (control hamster Ig), 68 (anti-α1), 29 (anti-α2), 18 (anti-α1 + anti-α2), 45 (anti-α4), 18 (anti-α5), 20 (anti-α6), and 10 (anti-β1). The mAbs used were: Ha4/8 (control hamster Ig group 2), Ha31/8 (anti-α1), Ha1/29 (anti-α2), PS/2 (anti-α4), 5H10-27 (anti-α5), GoH3 (anti-α6), and HMβ1-1 (anti-β1).

**Figure 3.** *Effect of anti-integrin mAbs on the effector phase of contact hypersensitivity.* FITC-sensitized mice were injected i.p. with the indicated mAbs 4 h prior to FITC challenge. Ear thickness was measured at baseline and 24 h later, and results shown as % increase in ear thickness ± SEM as illustrated in Example 3.

These data represent a summary of nine experiments with n = 74 (PBS), 60 (control hamster Ig), 26 (anti-ICAM-1), 44 (anti-α1), 44 (anti-α2), 38 (anti-α1 + anti-α2), 36 (anti-α4), 16 (anti-α5), 26 (anti-α4 + anti-α5), 24 (anti-α6), and 22 (anti-β1). The hamster mAbs used were: Ha4/8 (control hamster Ig group 2), Ha31/8 (anti-α1), Ha1/29 (anti-α2), HMβ1-1 (anti-β1), 3E2 (anti-ICAM-1); the rat mAbs used were: R35-95 and R35-38 (control rat IgG2a and rat IgG2b, respectively), PS/2 (anti-α4), 5H10-27 (anti-α5), GoH3 (anti-α6).

**Figure 4.** *Contact hypersensitivity responses in α1-deficient mice compared to wild-type mice.* FITC-sensitized mice were injected i.p. with indicated mAbs 4 h prior to FITC challenge. Ear thickness was measured at baseline and 24 h later, and results shown as % increase in ear thickness ± SEM as illustrated in Example 4. Groups of four to five mice per condition were used, and all experiments were performed a minimum of three times. One representative experiment is shown.

**Figure 5.** *Effect of anti-α1 and anti-α2 mAbs on croton oil-induced non-specific inflammation.* Mice were injected i.p. with indicated mAbs 4 h prior to ear painting with croton oil. Ear thickness was measured at baseline and 24 h later, and results shown as % increase in ear thickness ± SEM as illustrated in Example 5. Groups of four to five mice per condition were used, and all experiments were performed a minimum of three times. One representative experiment is shown.

**Figure 6.** *Effect of anti-α1 and α2 mAbs in collagen mAb-induced arthritis.* Mice were injected i.p. with anti-collagen mAbs at d 0, followed by LPS on day 3. Mice were injected i.p. with indicated mAbs every 3rd day starting on d 0. Clinical arthritis was apparent 2-3 d following LPS injection and continued for several weeks. Each limb was evaluated on a 0 to 4 scale every 3rd day as illustrated in Example 6 and results are expressed as the mean arthritic score between d 9 and d 15 (± SEM) of all four limbs. These data represent a summary of four experiments with each experiment consisting of groups of three to four mice per condition.

**Figure 7.** *Effect of anti-α1 and α2 mAbs in collagen mAb-induced arthritis.* A. Preventative treatment of mice with either anti-α1 or anti-α2 mAb decreases arthritic score. Mice were treated with anti-collagen mAbs at d 0, followed by LPS on d 3. Arthritis was apparent by d 6 and continued for several weeks. Mice

were treated with the indicated mAbs every 3rd day starting on d 0. Each limb was evaluated and scored on a 0 to 4 scale every 3rd day. Results are expressed as the mean arthritic score between d 9 and d 15 (± SEM) of all four limbs (maximum score of 16). Groups of 4 mice per condition were used; the average of 12 experiments is shown. B. α1-deficient mice have a reduced arthritic score comparable to anti-α1 mAb-treated wild-type mice. Experimental details and scoring are as outlined above. Groups of 4 mice per condition were used; the average of 2 experiments is shown.

**Figure 8.** Development of arthritis is delayed in the absence of lymphocytes and inhibition of arthritis by anti-α1 mAb occurs in the absence of lymphocytes. Wild-type B6,129 or RAG-1-deficient B6,129 mice were treated with anti-collagen mAbs at day 0, followed by LPS on day 3. Arthritis was apparent by day 6 and continued for several weeks. Mice were treated with the indicated mAbs every 3rd day starting on day 0. Each limb was evaluated and scored on a 0 to 4 scale every 3rd day. Results are expressed as the mean arthritic score per limb (maximum score of 4). Groups of 4 mice per condition were used.

**Figure 9.** Dose response of anti-α1 mAb inhibition of arthritis. Wild-type Balb/c mice were treated with anti-collagen mAbs at day 0, followed by LPS on day 3. Arthritis was apparent by day 6 and continued for several weeks. Mice were treated i.p. with the indicated dose of either Ha4/8 (isotype control) or Ha31/8 (anti-α1) mAbs every 3rd day starting on day 0. Each limb was evaluated and scored on a 0 to 4 scale every 3rd day. Results are expressed as the mean arthritic score per limb (maximum score of 4). Groups of 4 mice per condition were used.

**Figure 10.** Therapeutic treatment with anti-α1 mAb can decrease arthritic score. Wild-type Balb/c mice were treated with anti-collagen mAbs at day 0, followed by LPS on day 3. Arthritis was apparent by day 6 and continued for several weeks. Mice were treated i.p. with mAbs (250 μg) or Ig fusion protein (200 μg) every 3rd day starting on day 4. Mice received either mAb (Ha4/8 isotype control or Ha31/8 anti-α1), Ig fusion protein (Isotype control Ig or TNF-R55-Ig) or a combination of both (250 ug Ha31/8 and 200 ug TNF-R55-Ig). Each limb was evaluated and scored on a 0 to 4 scale every 3rd day. Results are expressed as the mean arthritic score per limb (maximum score of 4). Groups of 4 mice per condition were used.

**Figure 11.** *Location of the Epitope for the anti-α1 I domain Blocking mAbs.* A. Amino acid sequence of the rat (top; SEQ ID NO:63) and human (below; SEQ ID NO:64) α1-I domain. The residues that comprise the MIDAS (metal ion dependent adhesion site) motif are shown in bold. The human amino acids that replaced the corresponding rat residues (RΔH) are shown below the rat sequence in the boxed region. For clarity, residue numbering in the text refers to this figure, , unless otherwise designated, e.g., as crystal numbering. B. Increasing concentrations of mAb AJH10 (ATCC No. PTA-3580; deposited under the Budapest Treaty with the American Type Culture Collection, Manassas, VA, USA on August 2, 2001) were bound to plates coated with 30 μg/ml human (circles), rat (triangles) or RΔH (squares) α1-I domain. Data shown is representative of three experiments.

**Figure 12.** Amino acid sequence of the human α1-I domain (SEQ ID NO:64).

**Figure 13.** *Identification of a blocking mAb to the α1-I domain.* A. Increasing concentration of mAbs AEF3 (triangles) or AJH10 (circles) were bound to plates coated with 30 μg/ml α1- I domain. B. The α1-I domain was treated with increasing concentrations of mAb AJH10 (diamonds) or mAb BGC5 (squares) and bound collagen IV (2 μg/ml) coated plates. C. K562-α1 cell were treated with increasing concentration of mAbs AEF3(triangles) or AJH10 (circles) and bound to collagen IV (5 μg/ml) coated plates. 45-50% of cells added to each well adhered to collagen IV. Data shown is representative of three independent experiments.

**Figure 14.** *Species Cross-reactivity of the blocking mAbs* analyzed by fluorescence activated cell sorter (FACS). Rabbit vascular smooth muscle cells were incubated with either mAb AJH10 (bottom) or murine IgG control (top) and analyzed by fluorescence activated cell sorter (FACS).

**Figure 15.** *The α1-I domain binds collagen.* A. Increasing concentrations of the human α1-I domain were bound to plates previously coated with 1 μg/ml collagen I (squares) or collagen IV (circles). Values shown have been corrected for background binding to BSA. B. 2 μg/ml human α1-I domain was mixed with increasing concentration of an anti- human α1 integrin antibody 5E8D9 (squares) or an anti- human α2- integrin antibody A2IIE10 (circles), and then bound

to plates previously coated with 1 μg/ml collagen IV. C. Plates were coated with 1 μg/ml collagen IV or 3% BSA. α1-I domain (2 μg/ml) was subsequenctly bound to coated plates plates in the presence of 1 mM $Mn^{2+}$, 1 mM $Mg^{2+}$, or 5 mM EDTA. Data shown is representative of three independent experiments.

**Figure 16.** *Characterization of Humanized AQC2 Forms.* mAQC2 (triangles), chAQC2 (circles), hAQC2 (inverted triangles) and hAQC2' (squares) were evaluated.

A. Inhibition of VLA-1 binding to type IV collagen.

B. Inhibition of α1-I domain binding to type IV collagen.

C. Binding to immobilized α1-I domain.

D. Competition with biotinylated mAQC2 for binding to immobilized α1-I domain.

**Figure 17.** *Characterization of Humanized AQC2 Forms* by FACS.

**Figure 18.** *Characterization of Humanized AQC2 Forms* by FACS.

**Figure 19.** *Atomic structure coordinates for the α1-I domain/Fab complex*, as derived by X-ray crystallography from crystals of that complex in Protein Data Bank (PDB) format. The coordinates of the two complexes in the asymmetric unit are listed as follows.

Complex 1: molecule A = I domain of integrin
molecule H = heavy chain of hAQC2 Fab
molecule L = light chain of hAQC2 Fab
molecule M = $Mn^{+2}$

Complex 2: molecule B = I domain of integrin
molecule X = heavy chain of hAQC2 Fab
molecule Y = light chain of hAQC2 Fab
molecule M = $Mn^{+2}$

**Figure 20.** *I domain-Fab complex.* A. Ribbon diagram of the I domain-Fab complex. The I domain is colored green and the antibody heavy and light chain yellow and blue, respectively. The $Mn^{+2}$ ion is the white colored sphere. B. Close-up of the MIDAS (Metal-Ion-Dependent-Adhesion-Site) site showing the coordination of the metal ion (white sphere) by Asp101 (crystal numbering). The

protein backbones are shown as ribbons and the side chains in the ball-and-stick representation. The blue cylinders represent interactions between the metal ion and protein atoms. The thin lines represent H-bonds. Fig. 20 was made with the software program RIBBONS (Carson, 1991, *J. Appl. Cryst.* 24:958-961).

**Figure 21.** *A diagram of a system used to carry out the instructions encoded by the storage medium of Figs. 22 and 23.*

**Figure 22.** *A cross section of a magnetic storage medium.*

**Figure 23.** *A cross section of an optically-readable data storage medium.*

## DETAILED DESCRIPTION OF THE INVENTION

It is a discovery of the present invention that an antibody to an integrin (e.g., VLA-1) and fragment thereof, particularly, an α1-integrin subunit, can block the interaction of pro-inflammatory leukocytes with components of the extracellular matrix including, but not limited to collagens, laminin and fibronectin. This discovery illustrates the importance of adhesion molecules of the integrin family, particularly α1β1, in the peripheral tissue environment during conditions related to inflammation. It also extends the role of integrins family and fragments thereof in inflammation beyond leukocyte attachment and extravasation at the endothelial interface by highlighting the importance of the matrix-rich peripheral tissue environment to immune responses and it reveals peripheral tissues as a new point of intervention for adhesion based therapies.

### I. Anti-Integrin Antibodies

The methods of the present invention contemplate the use of antibodies to integrins where the integrins contemplated include molecules which comprise a β chain, including but not limited to β1, β2, β3, β4, β5, β6, β7, β8, non-covalently bound to an α chain, including but not limited to α1, α2, α3, α4, α5, α6, α7, α8, α9, α10, αV, αL, αM, αX, αD, αE, αIIb. Examples of the various integrins contemplated for use in the invention include, but are not limited to:

α1β1, α2β1, α3β1, α4β1, α5β1, α6β1, α7β1, α8β1, α9β1, α10β1, αVβ1, αLβ1, αMβ1, αXβ1, αDβ1, αIIbβ1, αEβ1;

α1β2, α2β2, α3β2, α4β2, α5β2, α6β2, α7β2, α8β2, α9β2, α10β2, αVβ2, αLβ2, αMβ2, αXβ2, αDβ2, αIIbβ2, αEβ2;

α1β3, α2β3, α3β3, α4β3, α5β3, α6β3, α7β3, α8β3, α9β3, α10β3, αVβ3, αLβ3, αMβ3, αXβ3, αDβ3, αIIbβ3, αEβ3;

α1β4, α2β4, α3β4, α4β4, α5β4, α6β4, α7β4, α8β4, α9β4, α10β4, αVβ4, αLβ4, αMβ4, αXβ4 αDβ4, αIIbβ4, αEβ4;

α1β5, α2β5, α3β5, α4β5, α5β5, α6β5, α7β5, α8β5, α9β5, α10β5, αVβ5, αLβ5, αMβ5, αXβ5, αDβ5, αIIbβ5, αEβ5;

α1β6, α2β6, α3β6, α4β6, α5β6, α6β6, α7β6, α8β6, α9β6, α10β6, αVβ6, αLβ6, αMβ6, αXβ6, αDβ6, αIIbβ6, αEβ6;

α1β7, α2β7, α3β7, α4β7, α5β7, α6β7, α7β7, α8β7, α9β7, α10β7, αVβ7, αLβ7, αMβ7, αXβ7, αDβ7, αIIbβ7, αEβ7;

α1β8, α2β8, α3β8, α4β8, α5β8, α6β8, α7β8, α8β8, α9β8, α10β8, αVβ8, αLβ8, αMβ8, αXβ8, αDβ8, αIIbβ8, αEβ8;

The methods of the present invention also contemplate the use of antibodies to integrin fragments including for example antibodies to a β chain alone, including but not limited to β1, β2, β3, β4, β5, β6, β7, β8, as well as an α chain alone, including but not limited to α1, α2, α3, α4, α5, α6, α7, α8, α9, α10, αV, αL, αM, αX, αD, αE, αIIb. In addition, the methods of the present invention further contemplate the use of antibodies to integrin fragments including for example

antibodies to the I domain of the α chain, including but not limited to the I domain from α1β1 (Briesewitz et al., 1993, *J. Biol. Chem.* 268:2989); α2β1 ( Takada and Hemler, 1989, *J Cell Biol* 109:397), αLβ2 (Larson et al., 1989, *J Cell Biol* 108:703), αMβ2 (Corbi et al., 1988, *J Biol Chem* 263:12403), αXβ2 (Corbi et al., 1987, *EMBO J* 6:4023), αDβ2 (Grayson et al., 1988, *J Exp Med* 188:2187), αEβ7 (Shaw et al., 1994, *J Biol Chem* 269:6016). In one embodiment, the α1-I domain antigenic determinant includes an amino acid sequence of at least 6 contiguous amino acids, wherein the contiguous sequence is found within the sequence of Fig. 12. In a related embodiment, the contiguous sequence is Val-Gln-Arg-Gly-Gly-Arg.

Methods for producing integrins for use in the present invention are known to those of skill in the art (see, e.g., Springer et al., 1990, *Nature* 346:425-434).

Embodiments of the present invention further include anti-integrin polyclonal and monoclonal antibodies. Embodiments of the present invention include a monoclonal antibody such an anti-α1monoclonal antibody. Antibodies for treatment, in particular for human treatment, include human antibodies, humanized antibodies, chimeric antibodies, and antigen-binding fragments of whole antibodies such as Fab, Fab', F(ab')2 and F(v) antibody fragments. Some antibodies of this invention may also include proteins containing one or more immunoglobulin light chains and/or heavy chains, such as monomers and homo-or hetero-multimers (e.g., dimers or trimers) of these chains, where these chains are optionally disulfide-bonded or otherwise cross-linked. These antibodies may be capable of binding to one or more antigens (e.g., α1, α2, α6 or alpha-I domain containing integrin subunits).

An α1β1function blocking antibody as used herein refers to an antibody that binds to the α1-I domain, for example, residues 92-97 of Fig. 12, and blocks α1β1function as tested, for example, by their ability to inhibit K562-α1 dependent adhesion to Collagen IV (see Example 15).

The following describes the various methods of making the antibodies of this invention. Methods that are known in the art but not specifically described herein are also within the scope of this invention. For instance, antibodies of this invention can also be identified using phage-displayed antibody libraries, such as those described in Smith, 1985, *Science* 228:1315-7; U.S. Patents 5,565,332,

5,733,743, 6,291,650, and 6,303,313. Additional antibodies of this invention can be made by coupling the heavy chains identified herein with a noncognate light chain, e.g., a light chain identified by phage display technology.

**II. Non-Human Hybridoma Antibodies**

The monoclonal antibodies of this invention can be generated by well known hybridoma technology. For instance, $\beta_1$ -/- animals (e.g., mice, rats or rabbits) can be immunized with purified or crude $\alpha_1\beta_1$ preparations, cells transfected with cDNA constructs encoding $\alpha_1$, $\beta_1$ or both antigens, cells that constitutively express $\alpha_1\beta_1$, and the like. The antigen can be delivered as purified protein, protein expressed on cells, protein fragment or peptide thereof, or as naked DNA or viral vectors encoding the protein, protein fragment, or peptide. Sera of the immunized animals are then tested for the presence of anti-$\alpha_1\beta_1$ antibodies. B cells are isolated from animals that test positive, and hybridomas are made with these B cells.

Antibodies secreted by the hybridomas are screened for their ability to bind specifically to VLA-1 (e.g., binding to $\alpha_1$-transfected cells and not to untransfected parent cells) and for any other desired features, e.g., having the desired CDR consensus sequences, inhibiting (or not inhibiting in the case of nonblockers) the binding between collagen and VLA-1.

Hybridoma cells that test positive in the screening assays are cultured in a nutrient medium under conditions that allow the cells to secrete the monoclonal antibodies into the culture medium. The conditioned hybridoma culture supernatant is then collected and antibodies contained in the supernatant are purified. Alternatively, the desired antibody may be produced by injecting the hybridoma cells into the peritoneal cavity of an unimmunized animal (e.g., a mouse). The hybridoma cells proliferate in the peritoneal cavity, secreting the antibody which accumulates as ascites fluid. The antibody may then be harvested by withdrawing the ascites fluid from the peritoneal cavity with a syringe.

The monoclonal antibodies can also be generated by isolating the antibody-coding cDNAs from the desired hybridomas, transfecting mammalian host cells (e.g., CHO or NSO cells) with the cDNAs, culturing the transfected host cells, and recovering the antibody from the culture medium.

III. Chimeric Antibodies

The monoclonal antibodies of this invention can also be generated by engineering a cognate hybridoma (e.g., murine, rat or rabbit) antibody. For instance, a cognate antibody can be altered by recombinant DNA technology such that part or all of the hinge and/or constant regions of the heavy and/or light chains are replaced with the corresponding components of an antibody from another species (e.g., human). Generally, the variable domains of the engineered antibody remain identical or substantially so to the variable domains of the cognate antibody. Such an engineered antibody is called a chimeric antibody and is less antigenic than the cognate antibody when administered to an individual of the species from which the hinge and/or constant region is derived (e.g., a human). Methods of making chimeric antibodies are well known in the art. Human constant regions include those derived from IgG1 and IgG4.

IV. Fully Human Antibodies

The monoclonal antibodies of this invention also include fully human antibodies. They may be prepared using *in vitro*-primed human splenocytes, as described by Boerner et al., 1991, *J. Immunol.* 147:86-95, or using phage-displayed antibody libraries, as described in, e.g., U.S. Patent 6,300,064.

Alternatively, fully human antibodies may be prepared by repertoire cloning as described by Persson et al., 1991 , *Proc. Nat. Acad. Sci. USA* 88: 2432-2436; and Huang and Stollar, 1991, *J. Immunol. Methods* 141: 227-236. In addition, U.S. Patent 5,798,230 (Aug. 25, 1998) describes preparation of human monoclonal antibodies from human B cells, wherein human antibody-producing B cells are immortalized by infection with an Epstein-Barr virus, or a derivative thereof, that expresses Epstein-Barr virus nuclear antigen 2 (EBNA2), a protein required for immortalization. The EBNA2 function is subsequently shut off, resulting in an increase in antibody production.

Some other methods for producing fully human antibodies involve the use of non-human animals that have inactivated endogenous Ig loci and are transgenic for un-rearranged human antibody heavy chain and light chain genes. Such transgenic animals can be immunized with $\alpha_1\beta_1$ and hybridomas are then made from B cells

derived therefrom. These methods are described in, e.g., the various GenPharm/Medarex (Palo Alto, CA) publications/patents concerning transgenic mice containing human Ig miniloci (e.g., Lonberg U.S. Patent 5,789,650); the various Abgenix (Fremont, CA) publications/patents with respect to XENOMICE (e.g., Kucherlapati U.S. Patents 6,075,181, 6,150,584 and 6,162,963; Green et al., 1994, *Nature Genetics* 7:13-21; and Mendez et al., 1997, *Nature Genetics* 15(2):146-56); and the various Kirin (Japan) publications/patents concerning "transomic" mice (e.g., EP 843 961, and Tomizuka et al., 1997, *Nature Genetics* 16:133-1443).

**V. Humanized Antibodies**

The monoclonal antibodies of this invention also include humanized versions of cognate anti-$\alpha_1\beta_1$ antibodies derived from other species. A humanized antibody is an antibody produced by recombinant DNA technology, in which some or all of the amino acids of a human immunoglobulin light or heavy chain that are not required for antigen binding (e.g., the constant regions and the framework regions of the variable domains) are used to substitute for the corresponding amino acids from the light or heavy chain of the cognate, nonhuman antibody. By way of example, a humanized version of a murine antibody to a given antigen has on both of its heavy and light chains (1) constant regions of a human antibody; (2) framework regions from the variable domains of a human antibody; and (3) CDRs from the murine antibody. When necessary, one or more residues in the human framework regions can be changed to residues at the corresponding positions in the murine antibody so as to preserve the binding affinity of the humanized antibody to the antigen. This change is sometimes called "back mutation." Humanized antibodies generally are less likely to elicit an immune response in humans as compared to chimeric human antibodies because the former contain considerably fewer non-human components.

The methods for making humanized antibodies are described in, e.g., Winter EP 239 400; Jones et al., 1986, *Nature* 321:522-525; Riechmann et al., 1988, *Nature* 332:323-327 (1988); Verhoeyen et al., 1988, *Science* 239:1534-1536; Queen et al., 1989, *Proc. Nat. Acad. Sci.* USA 86:10029; U.S. Patent 6,180,370; and Orlandi et al., 1989, *Proc. Natl. Acad. Sci.* USA 86:3833. Generally, the transplantation of murine (or other non-human) CDRs onto a human antibody is achieved as follows.

The cDNAs encoding heavy and light chain variable domains are isolated from a hybridoma. The DNA sequences of the variable domains, including the CDRs, are determined by sequencing. The DNAs encoding the CDRs are transferred to the corresponding regions of a human antibody heavy or light chain variable domain coding sequence by site directed mutagenesis. Then human constant region gene segments of a desired isotype (e.g, γ1 for CH and k for CL) are added. The humanized heavy and light chain genes are co-expressed in mammalian host cells (e.g., CHO or NSO cells) to produce soluble humanized antibody. To facilitate large scale production of antibodies, it is often desirable to produce such humanized antibodies in bioreactors containing the antibody-expressing cells, or to produce transgenic mammals (e.g., goats, cows, or sheep) that express the antibody in milk (see, e.g., U.S. Patent 5,827,690).

At times, direct transfer of CDRs to a human framework leads to a loss of antigen-binding affinity of the resultant antibody. This is because in some cognate antibodies, certain amino acids within the framework regions interact with the CDRs and thus influence the overall antigen binding affinity of the antibody. In such cases, it would be critical to introduce "back mutations" (*supra*) in the framework regions of the acceptor antibody in order to retain the antigen-binding activity of the cognate antibody.

The general approach of making back mutations is known in the art. For instance, Queen et al. (*supra*), Co et al., 1991, *Proc. Nat. Acad. Sci.* USA 88:2869-2873, and WO 90/07861 (Protein Design Labs Inc.) describe an approach that involves two key steps. First, the human V framework regions are chosen by computer analysis for optimal protein sequence homology to the V region framework of the cognate murine antibody. Then, the tertiary structure of the murine V region is modeled by computer in order to visualize framework amino acid residues that are likely to interact with the murine CDRs, and these murine amino acid residues are then superimposed on the homologous human framework.

Under this two-step approach, there are several criteria for designing humanized antibodies. The first criterion is to use as the human acceptor the framework from a particular human immunoglobulin that is usually homologous to

the non-human donor immunoglobulin, or to use a consensus framework from many human antibodies. The second criterion is to use the donor amino acid rather than the acceptor if the human acceptor residue is unusual and the donor residue is typical for human sequences at a specific residue of the framework. The third criterion is to use the donor framework amino acid residue rather than the acceptor at positions immediately adjacent to the CDRs.

One may also use a different approach as described in, e.g., Tempest, 1991, *Biotechnology* 9: 266-271. Under this approach, the V region frameworks derived from NEWM and REI heavy and light chains, respectively, are used for CDR-grafting without radical introduction of mouse residues. An advantage of using this approach is that the three-dimensional structures of NEWM and REI variable regions are known from X-ray crystallography and thus specific interactions between CDRs and V region framework residues can be readily modeled.

**VI. Other Moieties**

The monoclonal antibodies of this invention may further include other moieties to effect the desired functions. For instance, the antibodies may include a toxin moiety (e.g., tetanus toxoid or ricin) or a radionuclide (e.g., $^{111}In$ or $^{90}Y$) for killing of cells targeted by the antibodies (see, e.g., U.S. Patent 6,307,026). The antibodies may include a moiety (e.g., biotin, fluorescent moieties, radioactive moieties, histidine tag or other peptide tags) for easy isolation or detection. The antibodies may also include a moiety that can prolong their serum half life, for example, a polyethylene glycol (PEG) moiety, and a member of the immunoglobulin super family or fragment thereof (e.g., a portion of human IgG1 heavy chain constant region such as the hinge, CH2 and CH3 regions).

**VII. Crystallizable Compositions and Crystals**

This invention also provides a crystallizable composition containing a complex of: (1) a rat-human chimeric α1-I domain (e.g., mutant RΔH), or a portion thereof (e.g., a polypeptide including 135 to 336 amino acids of the rat-human chimeric α1-I domain); and (2) a Fab fragment of hAQC2, or a portion thereof (e.g., a polypeptide including 3 to 213 amino acids of the light chain and/or a polypeptide including 3 to 219 amino acids of the heavy chain). An exemplary complex is shown

in Fig. 20. The RΔH α1-I domain can include, e.g., amino acid residues 145 to 336 (crystal numbering) (SEQ ID NO:59, *infra*) of the rat α1 subunit. The hAQC2 Fab fragments may include light chain amino acid residues 1 to 106 (e.g., 1-213) of SEQ ID NO:3 and heavy chain amino acid residues 1 to 118 (e.g., 1-219) of SEQ ID NO:4. The hAQC2 Fab fragments may be obtained by papain digestion of the whole antibody or made by recombinant methods. The Fab fragments include at least an antigen-binding portion of the variable domains of the light chain and/or the heavy chains of hAQC2.

```
145  TQLDIV
151  IVLDGSNSIY PWESVIAFLN DLLKRMDIGP KQTQVGIVQY
191  GENVTHEFNL NKYSSTEEVL VAANKIVQRG GRQTMTALGI
231  DTARKEAFTE ARGARRGVKK VMVIVTDGES HDNYRLKQVI
271  QDCEDENIQR FSIAILGHYN RGNLSTEKFV EEIKSIASEP
311  TEKHFFNVSD ELALVTIVKA LGERIF
```

(SEQ ID NO:59)

Some crystallizable compositions and crystals of this invention may contain a molecule or molecular complex that is homologous to the α1-I domain and/or the hAQC2 Fab fragment by amino acid sequence or by three-dimensional structure. Examples of homologues include, but are not limited to: the α1-I domain and/or the hAQC2 Fab fragment with mutations, such as conservative substitutions, additions, deletions or a combination thereof. "Conservative substitutions" refer to replacement residues that are physically similar in size, shape, hydrophobicity, charge, and/or chemical properties to the corresponding reference residues. Methods for identifying a "corresponding" amino acid are known in the art and are based upon sequence, structural alignment, its functional position or a combination thereof as compared to the crystal structure solved in the present invention. For example, corresponding amino acids may be identified by superimposing the backbone atoms of the amino acids in the α1-I domain/hAQC2 complex and a α1-I domain and/or hAQC2 homologue using well known software applications, such as QUANTA (Molecular Simulations, Inc., San Diego, CA ©1998,2000). The corresponding

amino acids may also be identified using sequence alignment programs such as the "bestfit" program available from the Genetics Computer Group, which uses the local homology algorithm described by Smith and Waterman in *Adv. Appl. Math.* 2:482 (1981).

Crystallizable compositions of this invention may further include one or more components that promote crystallization and/or is compatible with crystallization conditions. Such components may include, but are not limited to, buffer, salts, precipitating agents and other reagents. One component can be 30% weight/volume Polyethylene Glycol 1500 (PEG1500).

The instant invention also provides methods of making crystals from crystallizable compositions including a complex of α1-I domain and an antigen-binding portion of hAQC2 (e.g., Fab, Fab' or other fragments, *supra*). Various techniques of crystallization can be used in the claimed invention, including, but not limited to, vapor-diffusion, dialysis, microbatch, batch, and liquid-liquid diffusion. Vapor diffusion methods include, but are not limited too, sitting-drop, hanging-drop and sandwich-drop techniques. Vapor-diffusion methods can use techniques to control the rate of crystallization, such as the addition of oils on the drops or reservoir solution. Crystallization methods can include mixing a reservoir solution containing precipitating agent with an aqueous solution of a complex of α1-I domain and an antigen-binding portion of hAQC2 to produce a crystallizable composition. The mixture or crystallizable composition may then be crystallized using the various above-listed techniques. The crystallizable composition of this invention may be an aqueous solution of a complex of α1-I domain and an antigen-binding portion of hAQC2 containing the complex at a concentration of about 1 to 50 mg per mL, such as a concentration of about 5 to 15 mg per mL (e.g., 11 mg per mL).

## VIII. Crystal Structures and Structure Coordinates

This invention further provides the three-dimensional structure of a crystal including a complex of mutant RΔH, and a hAQC2 Fab fragment at 2.8 Å resolution (Example 24, *infra*). The three-dimensional structures of other related crystals may also be determined using techniques described herein and those known in the art. The three-dimensional structure of this complex is defined by a set of

structure coordinates set forth in Fig. 19. These structure coordinates are Cartesian atomic coordinates derived from mathematical equations related to the patterns obtained from diffraction of a monochromatic beam of X-rays by the atoms or scattering centers of the crystalline complex of the α1-I domain and the hAQC2 Fab fragment. Diffraction data are first used to calculate an electron density map of the repeating unit of the crystal. The electron density map is then used to establish the positions of individual atoms of the complex.

This invention provides a molecule or a molecular complex defined by all or part of the structure coordinates of all amino acids set forth in Fig. 19, as well as a homologue of the molecule or molecular complex, where the homologue has a root mean square deviation from the backbone atoms of these amino acids between 0.00 Å and 0.65 Å, such as between 0.00 Å and 0.60 Å (e.g., between 0.00 Å and 0.50 Å). The term "root mean square deviation" or "r.m.s. deviation" means the square root of the arithmetic mean of the squares of the deviations from the mean. It is a way to express the deviation or variation from a trend or object. For purposes of this invention, the "root mean square deviation" or "r.m.s. positional deviation" defines the variation in the backbone of a protein from the relevant portion of the backbone of the polypeptide as defined by the structure coordinates described herein.

A molecule or a molecular complex of this invention may also include a binding site defined by structure coordinates of at least seven amino acids of the hAQC2 Fab fragment selected from the group including of light chain residues Asn30, Tyr48, Trp90, Ser91, Asn93 and Trp95, and heavy chain residues Ser30, Arg31, Trp47, Ser52, Gly53, His56, Tyr58, Phe99, Gly100 and Asp101 (crystal numbering) according to Fig. 19; or a homologue of the molecule or molecular complex, where the homologue includes a binding site that has a root mean square deviation from the backbone atoms of one or more of these amino acids between 0.00 Å and 1.10 Å, such as between 0.00 Å and 1.00 Å (e.g., between 0.00 Å and 0.50 Å). The term "binding site" as used herein, refers to a region of a molecule or molecular complex that, as a result of its shape and charge, favorably associates with another chemical entity. The term "site" includes, but is not limited to, trench, cleft, channel or pocket. For instance, binding sites on the α1-I domain may include a collagen-binding site

(Emsley et al., 1997, *supra*), an antibody-binding site, and an allosteric (or IDAS) binding site (Huth et al., 2000, *Proc. Natl. Acad. Sci. U.S.A.* 97:5231-5236). The term "chemical entity" includes, but is not limited to, any molecule, molecular complex, compound or fragment thereof. The term "associate with" refers to an association or binding in a condition of proximity between a chemical entity, or portions thereof, and a binding pocket or binding site on a protein. The association may be non-covalent -- where the juxtaposition is energetically favored by hydrogen bonding or van der Waals or electrostatic interactions -- or it may be covalent.

A molecule or molecular complex of this invention can include a binding site defined by structure coordinates of α1-I domain amino acids selected from the group consisting of residues Asp154, Ser156, Asn157, Ser158, Tyr160, Glu192, Gln218, Arg219, Gly220, Gly221, Arg222, Gln223, Thr224, Asp257, His261, Asn263, Arg291, and Leu294 (crystal numbering), according to Fig. 19, or a homologue of the molecule or molecular complex, where the homologue includes a binding site that has a root mean square deviation from the backbone atoms of the α1-I domain amino acids between 0.00 Å and 0.92 Å.

A molecule or molecular complex of this invention also may include a binding site defined by structure coordinates of α1-I domain amino acids selected from the group consisting of residues Glu192, Gln218, Arg219, Gly220, and Gly221 (crystal numbering), according to Fig. 19; or a homologue of the molecule or molecular complex, where the homologue includes a binding site that has a root mean square deviation from the backbone atoms of the α1-I domain amino acids between 0.00 Å and 0.30 Å.

Those of skill in the art will understand that a set of structure coordinates for a polypeptide is a relative set of points that define a shape in three dimensions. Thus, it is possible that an entirely different set of coordinates that define a similar or identical shape could be generated using mathematical manipulations of the structure coordinates in Fig. 19. For example, the structure coordinates could be manipulated by crystallographic permutations of the structure coordinates, fractionalization of the structure coordinates, integer additions or subtractions to sets of the structure coordinates, inversion of the structure coordinates, or any combination

thereof. Moreover, slight variations in the individual coordinates will have little effect on overall shape.

Alternatively, modification in the crystal structure due to mutations, such as additions, substitutions, and/or deletions of amino acids, or other changes in any of the polypeptide components (e.g., a hAQC2 Fab fragment or a αl-I domain) that make up the crystal can also account for variations in structure coordinates. If such variations are within an acceptable standard error as compared to the original coordinates, the resulting three-dimensional shape is considered to be the same as that of the unmodified crystal.

It is therefore necessary to determine whether an entity is sufficiently similar to all or parts of the structure described herein as to be considered the same. Such analyses may be carried out using current software applications, such as QUANTA (Accelrys, Inc. and Molecular Simulations, Inc., San Diego, CA ©1998,2000) and O (Jones et al., 1991, *Acta Cryst.* A47:110-119), and accompanying User Guides. The Molecular Similarity application of QUANTA and the LSQ application of O permit comparisons between different structures, different conformations of the same structure, and different parts of the same structure. The general procedure used in both applications is to input the structures to be compared, define the equivalent atomic positions in these structures, perform a fitting operation, and analyze the results.

When each structure is input into the application, it is given a name. and identified as the fixed structure or a moving structures. Atom equivalency is usually defined by equivalent atoms such as protein backbone atoms (N, Cα, C and O) for all conserved residues between the two structures being compared. The moving structure is translated and rotated to obtain an optimum or least-squares fit with the fixed structure. The root mean square difference of the fit over the specified pairs of equivalent atom is reported by both programs in angstroms.

For the purpose of this invention, any molecular complex that has a root mean square deviation of conserved residue backbone atoms (N, Cα, C, 0) between 0.00 Å and 1.50 Å, such as between 0.00 Å and 1.00 Å (e.g., between 0.00 Å and 0.50 Å), when superimposed on the relevant backbone atoms described by

structure coordinates listed in Fig. 19 are considered identical.

**IX. Determining Other Crystal Structures**

The structure coordinates set forth in Fig. 19 can also be used to aid in obtaining structural information about another crystallized molecular entity, such as another hAQC2 containing amino acid substitutions in one of its CDRs. This may be achieved by any well-known techniques, including molecular replacement, an especially useful method for determining the structures of mutants and homologues of α1-I domain/Fab.

The structure coordinates set forth in Fig. 19 can also be used for determining at least a portion of the three-dimensional structure of molecular entities that contain at least some structural features similar to at least a portion of the α1-I domain or the hAQC2 Fab. Therefore, another embodiment of this invention provides a method of utilizing molecular replacement to obtain structural information about a crystallized molecule or molecular complex with unknown structure including the steps of: (a) generating an X-ray diffraction pattern from the crystallized molecule or molecular complex; and (b) applying at least a portion of the structure coordinates set forth in Fig. 19 to the X-ray diffraction pattern to generate a three-dimensional electron density map of the molecule or molecular complex with unknown structure.

By using molecular replacement, all or part of the structure coordinates set forth in Fig. 19 can be used to determine the unknown structure of a crystallized molecular entity more rapidly and efficiently than attempting to determine such information *ab initio*. Molecular replacement provides an accurate estimation of the phases for an unknown structure. Phases are a factor in equations used to solve crystal structures that cannot be determined directly. Obtaining accurate values for the phases, by methods other than molecular replacement, can often be a time-consuming process that involves iterative cycles of approximations and refinements and greatly hinders the solution of crystal structures. However, when the crystal structure of a protein containing at least a homologous portion has been solved, the phases from the known structure can often provide a satisfactory estimate of the phases for the unknown structure.

Thus, molecular replacement involves generating a preliminary model

of a molecule or molecular complex whose structure coordinates are unknown, by orienting and positioning the relevant portion of the complex according to Fig. 19 within the unit cell of the crystal of the unknown molecule or molecular complex, so as best to account for the observed X-ray diffraction pattern of the crystal of the molecule or molecular complex whose structure is unknown. Phases can then be calculated from this model and combined with the observed X-ray diffraction pattern amplitudes to generate an electron density map of the structure whose coordinates are unknown. This, in turn, can be subjected to any well-known model building and structure refinement techniques to provide a final, accurate structure of the unknown crystallized molecule or molecular complex (Lattman, 1985, *Meth. Enzymol.* 115:55-77; Rossmann, ed., "The Molecular Replacement Method", Int. Sci. Rev. Ser., No. 13, Gordon & Breach, New York, 1972). The structure of any portion of any crystallized molecule or molecular complex that is sufficiently homologous to any portion of the α1-I domain and/or the hAQC2 Fab fragment (according to Fig. 19) can be solved by this method.

**X. Computer and Storage Medium**

To use the structure coordinates of this invention, e.g., those set forth in Fig. 19, it is usually necessary to convert the coordinates into a three-dimensional representation or shape. Commercially available graphical software programs including, but not limited to, O (Jones et al., 1991, *Acta Cryst.* A47:110-119) and INSIGHTII (© Accelrys, Inc. and Molecular Simulations, Inc., San Diego, CA) are capable of generating three-dimensional representations of molecules or molecular complexes, or portions thereof, from a set of structure coordinates.

In accordance with the present invention, the structure coordinates of the molecular entities of this invention are stored in a storage medium readable by machine (e.g., a computer). Using a computer and appropriate software, such data may be used for a variety of purposes, such as drug discovery and X-ray crystallographic analysis of other protein crystals.

Accordingly, a machine-readable data storage medium may include a data storage material encoded with machine-readable data including at least a portion of the structure coordinates set forth in Fig. 19. The computer may further include

instructions to produce three-dimensional representations of the molecular complexes of α1-I domain and the hAQC2 Fab fragment by processing the machine-readable data of this invention. The computer of this invention may also include a display, a graphical interface for displaying, or an input device for moving and manipulating the three-dimensional graphical representation of the structure coordinates.

This invention also provides a computer for determining at least a portion of the structure coordinates corresponding to X-ray diffraction data obtained from a molecular complex of α1β1 integrin and the Fab fragment of hAQC2 antibody, where the computer includes a machine-readable data storage medium including a data storage material encoded with machine-readable data, where the data includes at least a portion of the structure coordinates of the molecular complex of α1-I domain and the hAQC2 Fab fragment according to Fig. 19, or X-ray diffraction data obtained from the crystalline molecular complex. The computer further includes instructions for performing a Fourier transform of the machine readable coordinate data, and instructions for processing this machine readable diffraction data into structure coordinates. This computer may further include: a working memory for storing instructions for processing the machine-readable data; a central-processing unit coupled to the working memory and to the machine-readable data; and optionally a graphical interface or display coupled to the central-processing unit for displaying the three-dimensional graphical representation of the structure coordinates of the molecule or molecular complex.

This invention further provides a computer for producing a three-dimensional representation of: a molecule or a molecular complex defined by at least a portion or all of the structure coordinates of all the α1-I domain and the hAQC2 Fab fragment amino acids set forth in Fig. 19, or a homologue of the molecule or molecular complex, where the homologue has a root mean square deviation from the backbone atoms of the amino acids of between 0.00 Å than 1.50 Å, such as between 0.00 Å and 1.00 Å, (e.g., between 0.00 Å and 0.50 Å). Further in this invention the computer includes: a machine-readable data storage medium including a data storage material encoded with machine-readable data, where the data includes at least a portion or all of the structure coordinates of all of the α1-I domain and the Fab

hAQC2 fragment amino acids set forth in Fig. 19.

A computer of this invention may also produce a three-dimensional representation of a molecule or molecular complex including a binding site. The binding site may be defined by structure coordinates of at least seven amino acids of: the hAQC2 Fab fragment selected from the group including light chain residues Asn30, Tyr48, Trp90, Ser91, Asn93 and Trp95, and heavy chain residues Ser30, Arg31, Trp47, Ser52, Gly53, His56, Tyr58, Phe99, Gly100 and Asp101 (crystal numbering) according to Fig. 19; or a homologue of the molecule or molecular complex, where the homologue includes a binding site that has a root mean square deviation from the backbone atoms of the at least one amino acid of the hAQC2 Fab fragment of between 0.00 Å and 1.10 Å, such as between 0.00 Å and 1.00 Å, (e.g., between 0.00 Å and 0.50 Å). Further, the computer of this invention includes: a machine-readable data storage medium including a data storage material encoded with machine-readable data, where the data includes the structure coordinates of at least seven amino acids of the hAQC2 Fab fragment selected from the group consisting of light chain residues Asn30, Tyr48, Trp90, Ser91, Asn93 and Trp95, and heavy chain residues Ser30, Arg31, Trp47, Ser52, Gly53, His56, Tyr58, Phe99, Gly100 and Asp101 (crystal numbering) according to Fig. 19.

This invention also provides a computer for producing a three-dimensional representation of: a molecule or molecular complex including a binding site defined by structure coordinates I domain amino acids selected from the group consisting of residues Asp154, Ser156, Asn157, Ser158, Tyr160, Glu192, Gln218, Arg219, Gly220, Gly221, Arg222, Gln223, Thr224, Asp257, His261, Asn263, Arg291, and Leu294 (crystal numbering), according to Fig. 19; or a homologue of the molecule or molecular complex, where the homologue includes a binding site that has a root mean square deviation from the backbone atoms of the I domain amino acids between 0.00 Å and 0.92 Å. Further in this invention, the computer includes: a machine-readable data storage medium including a data storage material encoded with machine-readable data, where the data includes the structure coordinates of I domain amino acids selected from the group consisting of residues Asp154, Ser156, Asn157, Ser158, Tyr160, Glu192, Gln218, Arg219, Gly220, Gly221,

Arg222, Gln223, Thr224, Asp257, His261, Asn263, Arg291, and Leu294 (crystal numbering), according to Fig. 19.

This invention also provides a computer for producing a three-dimensional representation of a molecule or molecular complex including a binding site defined by structure coordinates of I domain amino acids selected from the group consisting of residues Glu192, Gln218, Arg219, Gly220, and Gly221 (crystal numbering), according to Fig. 19; or a homologue of the molecule or molecular complex, where the homologue includes a binding site that has a root mean square deviation from the backbone atoms of I domain amino acids between 0.00 Å and 0.30 Å. Further in this invention the computer includes: a machine-readable data storage medium including a data storage material encoded with machine-readable data, where the data includes the structure coordinates I domain amino acids selected from the group consisting of residues Glu192, Gln218, Arg219, Gly220, and Gly221 (crystal numbering), according to Fig. 19.

Fig. 21 demonstrates one such embodiment. System 10 includes a computer 11 including a central-processing unit ("CPU") 20, a working memory 22 which may be, e.g., RAM (random-access memory) or "core" memory, mass storage memory 24 (such as one or more disk or tape drives or CD-ROM or DVD-ROM drives), one or more cathode-ray tube ("CRT") display terminals 26, one or more keyboards 28, one or more input lines 30, and one or more output lines 40, all of which are interconnected by a conventional bidirectional system bus 50.

Input hardware 36, coupled to computer 11 by input lines 30, may be implemented in a variety of ways. Machine-readable data of this invention may be inputted via the use of a modem or modems 32 connected by a telephone line or dedicated data line 34. Alternatively or additionally, the input hardware 36 may include CD-ROM or DVD-ROM drives or tape or disk drives 24. In conjunction with display terminal 26, keyboard 28 may also be used as an input device.

Output hardware 46, coupled to computer 11 by output lines 40, may similarly be implemented by conventional devices. By way of example, output hardware 46 may include CRT display terminal 26 for displaying a graphical representation of a binding site of this invention using a program such as QUANTA as

described herein. Output hardware might also include a printer 42, so that hard copy output may be produced, or a disk drive 24, to store system output for later use.

In operation, CPU 20 coordinates the use of the various input and output devices 36, 46, coordinates data accesses from mass storage 24 and accesses to and from working memory 22, and determines the sequence of data processing steps. A number of programs may be used to process the machine-readable data of this invention. Such programs are discussed in reference to the computational methods of drug discovery as described herein. Specific references to components of the hardware system 10 are included as appropriate throughout the following description of the data storage medium.

Fig. 22 shows a cross-section of a magnetic data storage medium 100 which can be encoded with machine-readable data that can be carried out by a system such as system 10 of Fig. 21. Medium 100 can be a conventional floppy diskette or hard disk, having a suitable substrate 101, which may be conventional, and a suitable coating 102, which may be conventional, on one or both sides, containing magnetic domains (not visible) whose polarity or orientation can be altered magnetically. Medium 100 may also have an opening (not shown) for receiving the spindle of a disk drive or other data storage device 24.

The magnetic domains of coating 102 of medium 100 are polarized or oriented so as to encode in manner which may be conventional, machine readable data such as that described herein, for execution by a system such as system 10 of Fig. 21.

Fig. 23 shows a cross-section of an optically-readable data storage medium 110 which also can be encoded with such machine-readable data, or a set of instructions, which can be carried out by a system such as system 10 of Fig. 21. Medium 110 can be a conventional compact disk or DVD disk read only memory (CD-ROM or DVD-ROM) or a rewritable medium, such as a magneto-optical disk which is optically readable and magneto-optically writable. Medium 100 has a suitable substrate 111, which may be conventional, and a suitable coating 112, which may be conventional, usually of one side of substrate 111.

In the case of CD-ROM, as is well known, coating 112 is reflective and is impressed with a plurality of pits 113 to encode the machine-readable data. The

arrangement of pits is read by reflecting laser light off the surface of coating 112. A protective coating 114, which is substantially transparent, is provided on top of coating 112.

In the case of a magneto-optical disk, as is well known, coating 112 has no pits 113, but has a plurality of magnetic domains whose polarity or orientation can be changed magnetically when heated above a certain temperature, as by a laser (not shown). The orientation of the domains can be read by measuring the polarization of laser light reflected from coating 112. The arrangement of the domains encodes the data as described above.

**XI. Rational Drug Design**

The present invention permits the use of structure-based and rational drug design techniques to design, select, and synthesize or isolate chemical entities, such as inhibitors of the α1-I domain and to improve known inhibitors of this domain. These inhibitors may be capable of blocking the collagen-binding site of VLA-1. This invention also permits the use of structure-based and rational drug design techniques to design variants that may act as inhibitors of collagen binding.

The three-dimensional representation of this invention can be used experimentally or computationally to design potential inhibitors, other chemical entities, variants of the Fab fragment or combinations of chemical entities that may bind to and effect the biological functions of the hAQC2 Fab fragment or the chimeric α1-I domain of the current invention.

One skilled in the art can use one of several methods to screen chemical entities for their ability to associate with the complex of the hAQC2 Fab fragment or the chimeric α1-I domain of the current invention and more particularly with a binding site of either the I domain or the Fab fragment. This process may begin by visual inspection of, for example, the binding site for either the I domain or the Fab fragment on the computer screen, based on the coordinates of the complex in Fig. 19. Selected chemical entities may then be positioned in a variety of orientations, or docked, within an individual binding site of either the I domain or the Fab fragment. Docking may be accomplished using software such as QUANTA, followed by energy minimization and molecular dynamics with standard molecular mechanics forcefields,

such as CHARMM (Molecular Simulations, Inc., Burlington, MA ©1994) and AMBER (P.A. Kollman, University of California at San Francisco, ©1994).

Specialized computer programs may also assist in the process of selecting chemical entities. These include, *inter alia*:

1. GRID (Goodford, P.J., 1985, *J. Med. Chem.* 28:849-857). GRID is available from Oxford University, Oxford, UK.

2. MCSS (Miranker, A. and M. Karplus, 1991, *Proteins: Structure, Function and Genetics* 11:29-34). MCSS is available from Molecular Simulations, Burlington, MA.

3. AUTODOCK (Goodsell, D.S. and A.J. Olsen, 1990, *Proteins: Structure, Function, and Genetics* 8:195-202). AUTODOCK is available from Scripps Research Institute, La Jolla, CA.

4. DOCK (Kuntz, I.D. et al., 1982, *J. Mol. Biol.* 161:269-288). DOCK is available from University of California, San Francisco, CA.

Once suitable chemical entities have been selected, they can be assembled into a single compound. Assembly may proceed by visual inspection of the relationship of the entities to each other on the three-dimensional image displayed on a computer screen in relation to the structure coordinates of the complex of hAQC2 Fab fragment and the chimeric α1-I domain. This is followed by manual model building using software such as Quanta or Sybyl.

The above-described evaluation process for chemical entities may be performed in a similar fashion for compounds or for variants that may bind the α1-I domain.

Useful programs to aid one of skill in the art in connecting the individual chemical entities include:

1. CAVEAT (Bartlett, P.A. et al, "CAVEAT: A Program to Facilitate the Structure-Derived Design of Biologically Active Molecules". In "Molecular Recognition in Chemical and Biological Problems", Special Pub., 1989, Royal Chem. Soc., 78:182-196). CAVEAT is available from the University of California, Berkeley, CA.

2. 3D Database systems such as MACCS-3D (MDL Information Systems, San Leandro, CA). This area is reviewed in Martin, Y.C., 1992, *J. Med. Chem.* 35:2145-2154.

3. HOOK (available from Molecular Simulations, Burlington, MA).

Instead of proceeding to build an inhibitor or binding compound in a step-wise fashion one chemical entity at a time, as described above, binding compounds may be designed as a whole or "de novo" using either an empty binding site (such as a binding site of the α1-I domain or the hAQC2 Fab fragment) or optionally including some portion(s) of a known α1-I domain or the hAQC2 Fab fragment binding compound. These methods include:

1. LUDI (Bohm, H.-J., 1992, *J. Comp. Aid. Molec. Design* 6:61-78). LUDI is available from Biosym Technologies, San Diego, CA.

2. LEGEND (Nishibata, Y. and A. Itai, 1991, *Tetrahedron* 47:8985). LEGEND is available from Molecular Simulations, Burlington, MA.

3. LeapFrog (available from Tripos Associates, St. Louis, MO).

Other molecular modeling techniques may also be employed in accordance with this invention. See, e.g., Cohen, N.C. et al., 1990, *J. Med. Chem.* 33:883-894. See also Navia, M.A. and M.A. Murcko, 1992, *Curr. Opin. Struct. Biol.* 2:202-210.

Once an entity has been designed or selected by the above methods, the efficiency with which that entity may bind to the α1-I domain or the hAQC2 Fab fragment can be tested and optimized by computational evaluation. For example, a compound that has been designed or selected to function as a α1-I domain binding compound can traverse a volume not overlapping that occupied by the binding site when it is bound to the chimeric α1-I domain. An effective α1-I domain binding compound can demonstrate a relatively small difference in energy between its bound and free states (i.e., a small deformation energy of binding). Thus, the most efficient α1-I domain binding compound should be designed with a deformation energy of binding of not greater than about 10 kcal/mole, e.g., not greater than 7 kcal/mole. α1-I domain binding compounds may interact with the α1-I domain in more than one conformation that is similar in overall binding energy. In those cases, the deformation energy of binding is taken to be the difference between the energy of the free compound and the average energy of the conformations observed when the compound binds to the protein.

A compound designed or selected as binding to α1-I domain may be further computationally optimized so that in its bound state it would lack repulsive electrostatic interaction with the target protein. Such non-complementary (e.g., electrostatic) interactions include repulsive charge-charge, dipole-dipole and charge-dipole interactions. Specifically, the sum of all electrostatic interactions between the compound and the protein when the compound is bound to α1-I domain, should make a neutral or favorable contribution to the enthalpy of binding.

Specific computer software is available in the art to evaluate compound deformation energy and electrostatic interaction. Examples of programs designed for such uses include: Gaussian 92, revision C (M.J. Frisch, Gaussian, Inc., Pittsburgh, PA ©1992); AMBER, version 4.0 (P.A. Kollman, University of California at San Francisco, ©1994); QUANTA/CHARMM (Molecular Simulations, Inc., Burlington, MA ©1994); and Insight II/Discover (Biosysm Technologies Inc., San Diego, CA ©1994). These programs may be implemented, for instance, using a Silicon Graphics workstation. Other hardware systems and software packages will be known to those skilled in the art.

One other useful drug design technique enabled by this invention is iterative drug design. Iterative drug design is a method for optimizing associations between a protein and a compound (that compound includes an antibody) by determining and evaluating the three-dimensional structures of successive sets of protein/compound complexes. In iterative drug design, a series of crystals of a protein complexed with entities that bind the protein are obtained and then the three-dimensional structure of each molecular complex is solved. Such an approach provides insight into the associations between the proteins and other entities of each complex. This is accomplished by selecting chemical entities with inhibitory activity, obtaining crystals of these new complexes, solving the three-dimensional structure of the complexes, and comparing the associations between the new complexes and the previously solved complex. Associations within a complex can be optimized by observing how changes in the components of the complex affect associations.

In some cases, iterative drug design is carried out by forming successive complexes and then crystallizing each new complex. Alternatively, a

pre-formed protein crystal is soaked in the presence of another chemical entity, thereby forming a complex and obviating the need to crystallize each individual complex.

**XII. Pharmaceutical Compositions**

The pharmaceutical compositions of this invention contains one or more VLA-1 antagonists of the present invention (e.g., anti-VLA-1 antibodies and the small molecular VLA-1 antagonists identified by the above-described rational drug design methods), or pharmaceutically acceptable derivatives thereof. The compositions may further contain a pharmaceutically acceptable carrier, such as an adjuvant, a vehicle, a buffer, and a stabilizer.

The pharmaceutical compositions of this invention may be given orally, topically, intravenously, subcutaneously, intraperitoneally, intramuscularly, intramedullarily, intraarterially, intra-articularly, intra-synovially, intrasternally, intrathecally, intrahepatically, intraspinally, intracranially as desired, or just locally at sites of inflammation or tumor growth. The pharmaceutical compositions of this invention may also be administered by inhalation through the use of, e.g., a nebulizer, a dry powder inhaler or a metered dose inhaler, or by implantation of an infusion pump or a biocompatible sustained release implant into the subject.

The pharmaceutical compositions may be in the form of a sterile injectable preparation, for example a sterile injectable aqueous or oleaginous suspension. This suspension may be formulated according to techniques known in the art using suitable dispersing, wetting, and suspending agents. If given orally, the pharmaceutical compositions can be administered in form of capsules, tablets, aqueous suspensions or solutions. For topical applications, the pharmaceutical compositions may be formulated in a suitable ointment.

The dosage and dose rate of the VLA-1 antagonists of this invention effective to produce the desired effects will depend on a variety of factors, such as the nature of the disease to be treated, the size of the subject, the goal of the treatment, the specific pharmaceutical composition used, and the judgment of the treating physician. Dosage levels of between about 0.001 and about 100 mg/kg body weight per day, for example between about 0.1 and about 50 mg/kg body weight per day, of the active

ingredient compound are useful. For instance, an antibody of the invention will be administered at a dose ranging between about 0.01 mg/kg body weight/day and about 20 mg/kg body weight/day, e.g., ranging between about 0.1 mg/kg body weight/day and about 10 mg/kg body weight/day, and at intervals of every one to fourteen days. In another embodiment, the antibody is administered at a dose of about 0.3 to 1 mg/kg body weight when administered intraperitoneally. In yet another embodiment, the antibody is administered at a dose of about 5 to 12.5 mg/kg body weight when administered intravenously. In one embodiment, an antibody composition is administered in an amount effective to provide a plasma level of antibody of at least 1 mg/ml.

**XIII. Diseased Conditions And Animal Models**

The VLA-1 antagonists of the invention are useful in the treatment, including prevention, of $\alpha_1\beta_1$-mediated diseases such as those enumerated above. The treatments of this invention are effective on both human and animal subjects afflicted with these conditions. Animal subjects to which the invention is applicable extend to both domestic animals and livestock, raised either as pets or for commercial purposes. Examples are dogs, cats, cattle, horses, sheep, hogs and goats.

The efficacy of the VLA-1 antagonists of the invention can be tested in various animal models. For instance, useful psoriasis and arthritis models include those described in WO 00/72881. Kidney fibrosis models include those described in WO 99/61040, the Alport's syndrome kidney model described in Cosgrove et al., 2000, *Am. J. Path.* 157:1649-1659, and the SNF1 mouse model of lupus nephritis described in Kalled et al., 2001, *Lupus* 10:9-22. Vascular fibrosis models for restenosis include a rat carotid balloon injury model described in Smith et al., 1999, *Circ. Res.* 84:1212-1222. Lung fibrosis models for idiopathic pulmonary fibrosis and scleroderma-associated pulmonary fibrosis include a bleomycin-induced pulmonary fibrosis model described in Wang et al., 1999, *Thorax* 54:805-812. Liver cirrhosis models for hepatitis C- or alcohol-induced cirrhosis include the bile duct ligation model described in George et al., 1999, *Proc. Natl. Acad. Sci. USA* 96:12719-12724 and the CCL4-induced liver fibrosis model described in Shi et al., 1997, *Proc. Natl. Acad. Sci. USA* 94:10663-10668.

The efficacy of the treatments of this invention may be measured by a number of available diagnostic tools, including physical examination, blood tests, proteinuria measurements, creatinine levels and creatinine clearance, pulmonary function tests, chest X-rays, bronchoscopy, bronchoalveolar lavage, lung biopsy, plasma blood urea nitrogen (BUN) levels, observation and scoring of scarring or fibrotic lesions, deposition of extracellular matrix such as collagen, smooth muscle actin and fibronectin, kidney function tests, ultrasound, magnetic resonance imaging (MRI), and CT scan.

**XIV. Diagnostic Methods**

The antibodies of this invention can be used to diagnose diseased conditions associated with altered $\alpha_1\beta_1$ expression levels. A tissue sample from a subject, such as a tissue biopsy, body fluid sample or lavage (e.g., alveolar lavage), can be tested in an antigen capture assay, ELISA, immunohistochemistry assay, and the like using the antibodies. A tissue sample from a normal individual is used as control.

Practice of the present invention will employ, unless indicated otherwise, conventional techniques of cell biology, cell culture, molecular biology, microbiology, recombinant DNA, protein chemistry, and immunology, which are within the skill of the art. Such techniques are described in the literature. See, for example, *Molecular Cloning: A Laboratory Manual*, 2nd edition (Sambrook et al., Eds.), 1989; *Oligonucleotide Synthesis*, (M.J. Gait, Ed.), 1984; U.S. Patent 4,683,195 to Mullis et al.; *Nucleic Acid Hybridization*, (B.D. Hames and S.J. Higgins), 1984; *Transcription and Translation*, (B.D. Hames and S.J. Higgins), 1984; *Culture of Animal Cells* (R.I. Freshney, Ed.), 1987; *Immobilized Cells and Enzymes*, IRL Press, 1986; *A Practical Guide to Molecular Cloning* (B. Perbal), 1984; *Methods in Enzymology*, Volumes 154 and 155 (Wu et al., Eds.), Academic Press, New York; *Gene Transfer Vectors for Mammalian Cells* (J.H. Miller and M.P. Calos, Eds.), 1987; *Immunochemical Methods in Cell and Molecular Biology* (Mayer and Walker, Eds.), 1987; *Handbook of Experiment Immunology*, Volumes I-IV (D.M. Weir and C.C. Blackwell, Eds.), 1986; *Manipulating the Mouse Embryo*, 1986.

Unless otherwise defined, all technical and scientific terms used herein

have the same meaning as commonly understood by one of ordinary skill in the art to which this invention belongs. Exemplary methods and materials are described below, although methods and materials similar or equivalent to those described herein can also be used in the practice or testing of the present invention. All publications and other references mentioned herein are incorporated by reference in their entirety. In case of conflict, the present specification, including definitions, will control. The materials, methods, and examples are illustrative only and not intended to be limiting. Throughout this specification and claims, the word "comprise," or variations such as "comprises" or "comprising" will be understood to imply the inclusion of a stated integer or group of integers but not the exclusion of any other integer or group of integers.

The following Examples are provided to illustrate the present invention, and should not be construed as limiting thereof.

## EXAMPLES

### Chemical reagents

Fluorescein isothiocyanate (FITC) was purchased from Sigma Chemical Co. (St. Louis, MO). Croton oil was purchased from ICN Biochemicals (Aurora, OH). Whole sheep blood in Alsevers solution was obtained from East Acres Biologicals (Southbridge, MA). Type I rat tail collagen and type IV mouse collagen were purchased from Collaborative Research Inc. (Bedford, MA) and Gibco (Gaithersburg, MD), respectively.

Balb/c female mice of 6-8 weeks of age were purchased from Taconic (Germantown, NY) and the $\alpha 1\beta 1$ integrin-deficient mice on a Balb/c background were as previously described (3).

### Example 1

*Monoclonal Antibodies*. Function-blocking mAbs to murine antigens were prepared in an azide-free and low endotoxin format: Ha31/8 (hamster anti-CD49a; integrin $\alpha 1$) (Mendrick et al. 1995. *Lab. Invest.* 72:367-375), Ha1/29 (hamster anti-CD49b; integrin $\alpha 2$)( $\beta 1$) (Mendrick et al. 1995. *Lab. Invest.* 72:367-375; Mendrick, D.L. and D.M. Kelly 1993 *Lab. Invest.* 69:690-702), hamster group II

control mAb Ha4/8 (hamster anti-KLH)(Mendrick, D.L. and D.M. Kelly 1993 *Lab. Invest.* 69:690-702), and PS/2 (rat anti-CD49d; integrin α4β1 chain) (Miyake et al. 1991 *J. Exp. Med.* 173:599-607). In addition, the following function-blocking mAbs to murine antigens were purchased as no-azide/low endotoxin preparations from Pharmingen (San Diego, CA): HMβ1-1 (hamster anti-CD29; integrin β1chain) (Noto et al. 1995 *Int. Immunol.* 7:835-842), Ha2/5 (hamster anti-CD29; integrin β1chain)( Mendrick, D.L. and D.M. Kelly 1993 *Lab. Invest.* 69:690-702), 3E2 (hamster anti-CD54, ICAM-1)( Scheynius et al.1993 J. Immunol. 150:655-663), 5H10-27 (rat anti-CD49e; integrin α5)( Kinashi, T., and T.A. Springer. 1994. *Blood Cells*. 20:25-44), GoH3 (rat anti-CD49f; integrin α6)( Sonnenberg et al. 1987 *J. Biol. Chem.* 262:10376-10383), and the rat isotype control mAbs R35-95 (rat IgG2a) and R35-38 (rat IgG2b).

*Adhesion Assay*. Splenocytes from Balb/c mice were cultured with 20 ng/ml IL-2 for 7-12 d. Adhesion of cells to type I and type IV collagen was as previously described (Gotwals et al. 1996 *J. Clin. Invest.* 97:2469-2477). Briefly, 96-well Maxisorp plates (Nunc, Napierville, IL) were coated with either 10 μg/ml type IV or 5 μg/ml type I collagen and non-specific sites blocked with 1% BSA. IL-2 activated splenocytes were labeled with 2 μM BCECF [2',7'-bis(carboxyethyl)-5(6) carboxyl fluorescein penta acetoxymethylester](Molecular Probes, Eugene, OR) and incubated with 10 μg/ml of indicated mAbs for 15 min. $10^5$ cells in 0.25% BSA in RPMI were then added to coated wells and incubated for 60 min at 37°C. Unbound cells were removed by washing three times with 0.25% BSA in RPMI. Adhesion was quantified using a CytoFluor 2350 fluorescent plate reader (Millipore, Bedford, MA). The ratio of bound cells to input cells was measured and percent adhesion relative to control mAb-treated cells (normalized to 100%) calculated. Background values due to cell adhesion on wells coated with BSA alone were subtracted.

*Expression and functional blockade of α1β1 and α2β1 on activated leukocytes*. Given the key role leukocytes play in inflammation, we decided to test whether anti-α1 and anti-α2 mAbs were capable of blocking leukocyte adhesion to collagens. In order to obtain leukocytes expressing high levels of both α1 and α2, murine T cells were stimulated *in vitro* with IL-2 for 7-12 d. These cells expressed

high levels of both α1 and α2 (Fig. 1A), and bound well to both collagen type IV and type I-coated surfaces (Fig. 1B). Adhesion to type IV collagen was partially inhibited by anti-α1 mAb alone and was not inhibited by anti-α2 mAb alone. In contrast, adhesion to type I collagen was completely inhibited by anti-α2 mAb and anti-α1 mAb alone showed only partial inhibition. Both anti-β1 mAb and the combination of anti-α1 and anti-α2 mAbs completely inhibited adhesion to types I and IV collagen. Having demonstrated that the α1β1 and α2β1 integrins are expressed on activated T cells and that anti-α1 and α2 mAbs are able to functionally block leukocyte adhesion to collagens, we used these mAbs to investigate the *in vivo* role of these integrins in animal models of inflammatory disorders.

**Example 2**

*Inhibition of DTH responses by anti-integrin mAbs.* SRBC-induced delayed type hypersensitivity (DTH) responses were adapted from a previously published protocol (Hurtrel et al., 1992, *Cell. Immunol.* 142:252-263). Briefly, mice were immunized s.c. in the back with 2 x $10^7$ SRBC in 100 ul PBS on d 0. The mice were challenged on d 5 by injecting 1 x $10^8$ SRBC in 25 ul PBS s.c into the right hind footpad. Footpad thickness was measured with an engineer's caliper (Mitutoyo/MTI, Paramus, NJ) 20 h after antigen challenge, and the degree of footpad swelling calculated. Results are reported as the mean percent increase footpad thickness ± SEM and calculated as % increase = [1- (Right footpad thickness 20 h after antigen challenge/Uninjected left footpad thickness 20 h after antigen challenge)] x 100. To block the effector phase of the SRBC-induced DTH response, therapeutic or control mAb (100 ug), which were prepared according to the methods described in Example 1, was given i.p. 1 h prior to antigen challenge on d 5.

SRBC-induced DTH is a well characterized *in vivo* model of inflammation, and in particular psoriasis, that has been used to demonstrate the importance of a variety of cytokines and adhesion molecules in inflammation (Tedder et al., 1995, *J. Exp. Med.* 181:2259-2264, Terashita et al., 1996, *J. Immunol.* 156:4638-4643). SRBC-sensitized mice received anti-integrin mAbs 1 h prior to footpad antigen challenge and inflammation was assessed 20 h later as measured by increased footpad thickness. PBS and control hamster Ig-treated mice showed a 60-

70% increase in footpad thickness 20 h after antigen challenge (Fig. 2). Compared to control hamster Ig treatment, anti-α1 or anti-α2 mAbs resulted in a 68% and 60% inhibition in footpad thickness, respectively. The combination of anti-α1 and α2 mAbs resulted in 71% inhibition, demonstrating little additive effect over anti-α1 or anti-α2 mAbs alone. Treatment with other anti-integrin mAbs was also effective at inhibiting DTH effector response. The degree of inhibition seen with the various mAb treatments was 49% (anti-α4), 23% (anti-α5), and 57% (anti-α6). Lastly, mAb blockade of the common β1 integrin subunit (mAb HMBI-1) inhibited the effector DTH response by 67%.

**Example 3**

*Inhibition of CHS effector responses by anti-integrin mAbs.* Contact hypersensitivity (CHS) to FITC was assayed as previously described (Gaspari et al., 1991, *In* Current Protocols in Immunology. J.E. Coligan, A.M. Kruisbeek, D.H. Margulies, E.M. Shevach, and W. Strober, editors. John Wiley & Sons, New York. Section 4.2:1). Briefly, mice were sensitized by painting 100 ul 0.5% FITC in 1:1 acetone/dibutylphthalate onto the shaved back on d 0. 10 d later, animals were challenged by applying 5 ul 0.5% FITC onto both sides of each ear. Ear swelling response was determined by ear thickness measured with an engineer's caliper (Mitutoyo/MTI, Paramus, NJ) at the time of antigen challenge (d 10) and 24 h later, and the results reported as mean percent increase in baseline ear thickness ± SEM. Increase in ear thickness was calculated as % increase = [1- (Ear thickness 24 h after antigen challenge/Ear thickness at the time of antigen challenge)] x 100. To block the effector phase of the CHS response, therapeutic or control mAb (250 ug) was given i.p. 4 h prior to antigen challenge on d 10. Mice that were antigen-sensitized and ear challenged with vehicle only (vehicle control) or mice that were ear challenged without prior sensitization (irritant control) served as negative controls (never exceeded 2% increase in ear thickness).

Given that CHS is mechanistically distinct from DTH and involves different effector cells, we investigated what effect anti-integrin mAbs had on the effector phase of the CHS response. Mice were hapten-sensitized using FITC applied to their shaved backs, followed 10 d later with FITC challenge to the ear resulting in

an inflammatory response the next day. FITC-sensitized mice demonstrated a 60-70% increase in thickness 24 h after antigen challenge (Fig. 3). Consistent with published results (Scheynius et al., *J. Immunol.* 150:655-663), anti-ICAM-1 mAb treatment resulted in 51% inhibition of ear swelling. Compared to control hamster mAb, treatment of mice with anti-α1 or anti-α2 mAb 4 h prior to antigen challenge resulted in 37% and 57% inhibition in ear swelling, respectively (Fig. 3). The combination of anti-α1 and anti-α2 mAbs resulted in slightly greater inhibition of ear swelling (65%). Treatment with other mAbs to β1 integrins revealed that while anti-α4 and anti-α5 mAbs resulted in no inhibition of FITC-induced CHS effector response when compared to control rat mAb, treatment with anti-α6 mAb resulted in an 86% inhibition of effector responses. Lastly, mAb blockade of the common β1 integrin subunit inhibited CHS effector responses by 74%. Similar CHS results were obtained using different strains of mice (C57/BL6, 129/Sv) and a different sensitizing agent (oxazolone) (data not shown). Similar to the results seen in the SRBC-induced DTH model, histologic analysis of inflammed ears revealed that both edema formation and leukocytic infiltration were inhibited by anti-α1 and anti-α2 mAb treatment.

Consistent with the finding that α1β1 and α2β1 can be expressed on IL-2-activated splenocytes, analysis of lymph nodes from antigen-sensitized mice (FITC or oxazolone) revealed α1β1 and α2β1 to be expressed exclusively on $CD44^{hi}$ $LFA\text{-}1^{hi}$ activated CD4+ and CD8+ T cells (data not shown). Treatment of mice with anti-α1 and anti-α2 mAbs did not result in deletion of these cells, as the numbers of activated T cells in both spleen and lymph nodes seen in response to antigen sensitization in the CHS model was unaffected. In addition, effector cells were not functionally deleted as prolonged treatment of antigen-sensitized mice with anti-α1 and anti-α2 mAbs (d 10-16) did not affect the inflammatory response of mice challenged with antigen at d 20 (data not shown).

Example 4

*CHS effector responses are decreased in α1β1-deficient mice.* To exclude the possibility that the inhibitory role of α1β1 in the effector response of FITC-mediated CHS was mAb-mediated, experiments were carried out in wild-type and α1β1-integrin deficient mice (Fig. 4). MAb inhibition of the effector phase in

wild-type mice was consistent with previous results, with 56% inhibition in ear thickness seen with anti-α1, 56% with anti-α2, and 62% with a combination of anti-α1 and anti-α2. The effector phase of CHS was significantly reduced in untreated α1β1-deficient mice as compared to untreated wild-type mice (30% vs 71% increase in ear thickness, respectively). As expected, the level of ear swelling in untreated α1β1-deficient mice was equivalent to the level of ear swelling seen in anti-α1 mAb-treated wild-type mice. Lastly, mAb blockade of α2β1 in the α1β1-deficient mice resulted in only slightly increased inhibition of ear swelling, consistent with the results seen in wild-type mice treated with a combination of anti-α1 and anti-α2 mAbs.

**Example 5**

To further exclude the possibility that the inhibitory effect of the anti-integrin mAbs seen in both the DTH and CHS models of inflammation is caused by a general anti-inflammatory effect mediated by the anti-α1 and anti-α2 mAbs, the effect of these mAbs on irritant dermatitis was studied.

To assess irritant dermatitis, mice were painted with 5 ul of 0.8% croton oil in acetone on both sides of each ear. Therapeutic or control antibodies were given 4 h prior to the application of the irritant. Ear swelling was measured 24 h later as described above and compared to ear thickness prior to croton oil application. Results are reported as mean percent increase in baseline ear thickness ± SEM as described above. Mice painted with acetone only (vehicle control) served as a negative control.

24 h later, ears of mice treated with croton oil showed a significant increase in ear thickness (48%), when compared to mice receiving vehicle only (acetone). Toxic ear swelling caused by croton oil was not significantly affected in mice pretreated with anti-α1 or anti-α2 mAbs when compared to either PBS or control mAb-treated animals (Fig. 5). Histologic examination of the croton oil-treated ears revealed no differences in numbers or types of infiltrating cells or edema formation in mice treated with anti-α1 or anti-α2 mAbs, as compared to control mAb-treated mice or PBS-treated mice (data not shown).

**Example 6**

*Inhibition of arthritis by α1β1 and α2β1.* As α1β1 is well expressed on infiltrating cells in the synovium of arthritis patients, we decided to examine whether anti-α1 or anti-α2 mAbs would be inhibitory in an accelerated model of arthritis previously described (Terato et al., 1992, *J. Immunol.* 148:2103-2108; Terato et al., 1995, *Autoimmunity* 22:137-147).

Arthrogen-CIA Antibody kits were purchased from Stratagene (La Jolla, CA) and arthritis induced using a well established protocol (Terato et al., 1992, *J. Immunol.* 148:2103-2108; Terato et al., 1995, *Autoimmunity* 22:137-147). Briefly, arthritis was induced through i.p. injection of a cocktail of 4 anti-collagen type II mAbs ( 1 mg each) on d 0, followed by i.p. injection of 50 ug LPS on d 3. Over the course of the next 3-4 d, the mice developed swollen wrists, ankles and digits. Therapeutic or control mAb (250 ug) was administered i.p. 4 h prior to injection of the anti-collagen mAbs on d 0, and again 4 h prior to LPS administration on d 3, and then continuing every 3rd day for the length of the experiment. Beginning on d 3, mice were evaluated for the development of arthritis. Severity of arthritis in each limb was scored using a four point system. 0=normal; 1=mild redness, slight swelling of ankle or wrist; 2=moderate swelling of ankle or wrist; 3=severe swelling including some digits, ankle, and foot; 4=maximally inflamed.

Severe arthritis in Balb/c mice developed within 72 h after LPS injection and persisted for more than 3 weeks. Neither injection of anti-collagen mAbs alone nor LPS alone induced arthritis. Mice receiving control mAb treatment displayed equally severe arthritis as than seen in PBS-treated mice (Fig. 6). In contrast, treatment with anti-α1 mAb alone resulted in a marked reduction (78%) in arthritis, lasting the duration of the experiment. Treatment with anti-α2 mAb alone also had a beneficial effect, resulting in a 32% decrease in the arthritic score as compared to control mAb-treated mice. The combination of anti-α1 and anti-α2 mAbs resulted in a similar degree of inhibition as seen with anti-α1 mAb alone.

**Example 7**

*Histological analysis of effect of anti-α1 and anti-α2 mAb treatment on the inflammatory cellular infiltrate.* Further histological analysis of the SRBC-induced DTH response confirmed the ability of anti-α1 and anti-α2 mAb treatment to modulate the elicited inflammatory response. An unchallenged footpad from an SRBC-sensitized mouse showed virtually no inflammatory cellular infiltrate when compared to an SRBC-challenged footpad from the same mouse. Treatment of SRBC-sensitized mice with anti-α1 and anti-α2 mAbs either alone or combined greatly reduced the number of these infiltrating cells found in SRBC-challenged footpads when compared to control mAb-treated mice. Closer examination of the infiltrating cells revealed most cells to be composed of neutrophils, with some monocytes and lymphocytes present, and confirmed that anti-α1 and anti-α2 mAb treatment greatly decreased the numbers of these cells.

**Example 8**

*Immunohistochemical demonstration of α1-expressing cells in the inflammatory cellular infiltrate.* Immunohistochemistry was performed to more precisely determine the nature of the infiltrating cells and whether they express collagen-binding integrins. Infiltrating cells from an inflamed footpad of an untreated mouse were examined for expression of α1β1 integrin and cell lineage markers. α1β1 integrin was found to be expressed on many infiltrating leukocytes. Dual immunohistochemistry was utilized to identify the nature of the infiltrating cells and the distribution of α1β1 expression. Using cell lineage markers, the infiltrate was found to be composed largely of granulocyte/monocytes (Mac-1+), with many of these cells being neutrophils (Gr1+), along with a smaller number of T lymphocytes (CD3+). Expression of α1 β1 integrin was found among all three subsets of cells, with α1 expressed on a subset of Mac-1+ granulocyte/monocytes, a subset of Gr1+ neutrophils, and on the majority of infiltrating CD3+ T lymphocytes. Detailed immunohistochemical analysis revealed that although anti-α1 and anti-α2 mAb treatment reduced the numbers of infiltrating cells, no change in the cellular composition of the infiltrate was seen (data not shown). Immunohistochemistry

staining with a FITC anti-hamster mAb confirmed the ability of the anti-α1 and anti-α2 mAb to localize to the inflamed footpad (data not shown).

Example 9

*Inhibition of arthritis by mAbs to α1β1 and α2β1 and in α1-deficient mice.* As α1β1 is well expressed on infiltrating cells in the synovium of arthritis patients, we decided to examine whether anti-α1 or anti-α2 mAbs would be inhibitory in an accelerated model of arthritis previously described (Terato et al., 1992, *J. Immunol* 148:2103-2108; Terato et al., 1995, *Autoimmunity* 22:137-147). This model involves injection of a cocktail of anti-collagen type II mAbs into mice, followed later by LPS administration, resulting in the development of arthritis over the next 3-7 d. Mice were given mAb every 3rd day starting at d 0, and scored for the development of arthritis every 3rd day. Severe arthritis developed in all mice within 72 h after LPS injection and persisted for more than 3 weeks. Neither injection of anti-collagen mAbs alone nor LPS alone induced arthritis. Mice receiving control mAb treatment displayed equally severe arthritis as than seen in PBS-treated mice (Fig. 7). In contrast, treatment with anti-α1 mAb alone resulted in a marked reduction (79% and higher) in arthritis, lasting the duration of the experiment. Treatment with anti-α2 mAb alone also had a beneficial effect, resulting in a 37% decrease in the arthritic score as compared to control mAb-treated mice. The combination of anti-α1 and anti-α2 mAbs resulted in a similar degree of inhibition as seen with anti-α1 mAb alone. Reduction of arthritic score with anti-α1 mAb treatment was seen in all mice and compares favorably with several other mAb-based treatments for arthritis such as soluble TNF receptor Ig fusion protein (Mori et al., 1996, *J. Immunol.* 157:3178-3182), anti-Mac-1 (Taylor et al., 1996, *Immunology.* 88:315-321), anti-α4 (Seiffge, 1996, *J. Rheumatol.* 23:2086-2091), and anti-ICAM-1 (Kakimoto et al., 1992, *Cell Immunol.* 142:326-337). In agreement with mAb-based data showing an important role for α1β1 in arthritis, untreated α1-deficient mice showed significant reduction in arthritic score when compared to wild-type mice.

**Example 10**

*Effect of anti-α1 mAb treatment on the immunopathology of arthritic joints*. Joints from wild-type arthritic mice (day 8) receiving either control mAb or anti-α1 mAb treatment were compared visually and histologically to joints from a normal untreated mouse. Visually, joints from control mAb-treated mice demonstrated redness and swelling of the entire foot including digits, while anti-α1 mAb-treated mice showed little if any signs of inflammation in either joints or digits. Histologic examination showed severe changes in control mAb-treated arthritic joints, with extensive infiltration of the subsynovial tissue with inflammatory cells, adherence of cells to the joint surface, and marked cartilage destruction as evidenced by proteoglycan loss. Consistent with previous reports (Terato et al., 1992, *J. Immunol* 148:2103-2108; Terato et al., 1995, *Autoimmunity* 22:137-147), the majority of the infiltrating cells in this model are neutrophils. Anti-α1 mAb treatment of mice dramatically reduced the amount of inflammatory infiltrate and the degree of cartilage destruction.

**Example 11**

*Development of arthritis is delayed in the absence of lymphocytes and inhibition of arthritis by anti-α1 mAb occurs in the absence of lymphocytes.* To determine what cell types might be important in the collagen mAb-induced arthritis model we compared the ability of wild-type B6-129 mice and RAG-1-deficient B6-129 mice to develop arthritis (Fig. 8). Genetic deletion of the RAG-1 (recombination activating gene-1) gene results in a complete loss of mature T and B lymphocytes (Mombaerts et al., 1992, *Cell* 68:869-877). Both the wild-type and RAG-1-deficient mice developed arthritis, though the kinetics of induction in the RAG-1-deficient mice is significantly slower (Fig. 8). These results suggest that while lymphocytes are involved in this model of arthritis, they are not required for the development and progression of the disease. Published reports examining the effect of the RAG-1-deficient mice in other models of arthritis also found that loss of T and B lymphocytes delayed the onset of arthritis (Plows et al., 1999, *J. Immunol.* 162:1018-1023). Treatment of either wild-type or RAG-1-deficient mice with anti-α1 mAb completely inhibited arthritis (Fig. 8). These results demonstrate that the effectiveness of anti-α1

mAb in this model is not dependent on the presence of lymphocytes, and that as suggested by previous experiments (Fig. 7), the efficacy of anti-α1 mAb in preventing disease may be through its action on other α1-expressing cells, such as macrophages and neutrophils.

**Example 12**

*Dose response of anti-α1 mAb inhibition of arthritis.* Given the striking effects of anti-α1 mAb treatment on preventing arthritis, we extended these studies to include a dose response analysis (Fig. 9). Different doses of mAb were admininstered i.p. every 3rd day starting at day 0. In agreement with earlier data, a 250 ug dose of anti-α1 mAb resulted in near complete prevention of arthritis. A lower dose of 100 ug of anti-α1 mAb was partially effective at preventing arthritis in this model, while lower doses did not have any discernable effect on arthritic score (Fig. 9).

**Example 13**

*Therapeutic treatment with anti-α1 mAb can decrease arthritic score.* Given the effectiveness of anti-α1 mAb in preventing arthritis, we attempted to treat mice that are on their way to develop disease. Arthritis was induced in mice by injection of a cocktail of anti-collagen type II mAbs on day 0, followed by LPS administration on day 3. Mice were then treated with either anti-α1 mAb or a soluble TNF receptor Ig fusion protein starting on day 4. Progression of arthritis was completely blocked in mice receiving anti-α1 mAb starting at day 4, when compared to mice receiving control hamster mAb starting at day 4 (Fig. 10). The degree of inhibition seen with therapeutic administration of anti-α1 mAb was complete and was equal to that seen with preventative treatment of anti-α1 mAb (started at day 0) (Fig. 10). In comparison, treatment with TNF receptor Ig fusion protein from day 4 onwards resulted in only a 60-70% inhibition in arthritic score when compared to control Ig fusion protein (Fig. 10). Combined treatment of anti-α1 mAb and TNF receptor Ig fusion together was effective at completely inhibiting arthritic score, which is not surprising given the complete effectiveness of anti-α1 mAb treatment alone in suppressing arthritis. In summary, these results indicate that therapeutic treatment

with anti-α1 mAb is effective at inhibiting arthritic score, and compares favorably to therapeutic treatment with a TNF antagonist.

**Example 14**

*Cloning and mutagenesis of the α1-I domain.* Human and rat α1β1 integrin I domain sequences were amplified from full length cDNAs (Kern, et al., 1994, *J. Biol. Chem.* 269, 22811-22816; Ignatius et al., 1990, *J. Cell Biol.* 111, 709-720) by the polymerase chain reaction (PCR) (PCR CORE Kit; Boehringer Mannheim, GmbH Germany), using either human specific primers, 5'-CAGGATCCGTCAGCCCCACATTTCAA-3' [forward] (SEQ ID NO:7), and 5'-TCCTCGAGGGCTTGCAGGGCAAATAT-3' [reverse] (SEQ ID NO:8), or rat specific primers, 5'-CAGGATCCGTCAGTCCTACATTTCAA-3' [forward] (SEQ ID NO:9), and 5'-TCCTCGAGCGCTTCCAAAGCGAATAT-3' [reverse] (SEQ ID NO:10).

The resulting PCR amplified products were purified, ligated into pGEX4t-i (Pharmacia), and transformed into competent DH5α cells (Life Technologies). Ampicillin resistant colonies were screened for the expression of the ~45 kDa glutathione S-transferase-I domain fusion protein. The sequences from inserts of plasmid DNA of clones that were selected for further characterization were confirmed by DNA sequencing.

A rat/human chimeric α1-I domain (RΔH) was generated (MORPH Mutagenesis kit; 5 prime – 3 prime), exchanging the rat residues G92, R93, Q94, and L97 (Fig. 11) for the corresponding human residues, V, Q, R, and R, respectively. Clones harboring the RΔH I domain were identified by the loss of a diagnostic Stu 1 restriction enzyme site, and the inserts confirmed by DNA sequencing. The amino acid sequence of the human α1-I domain is shown in Fig. 12.

**Example 15**

*Generation of mAbs specific to the α1-I domain.* Monoclonal antibodies have proved to be very useful probes in studying the relationship between structure and function of integrin subunits. For example, mAbs were used extensively to study regions of the β1 subunit associated with an activated conformation (Qu, A., and Leahy, D. J. (1996) *Structure* 4, 931-942). Thus, to identify potential probes for

conformational changes of the α1-I domain, we generated a panel of mAbs to the human α1-I domain.

Generation of anti-α1 I domain Monoclonal Antibodies. Female Robertsonian mice (Jackson Labs) were immunized intraperitoneally (i.p.) with 25 μg of purified human α1β1 (Edwards et al., 1995, *J. Biol. Chem.* 270, 12635-12640; Gotwals et al., 1999, *Biochemistry* 38:8280-8) emulsified with complete Fruend's adjuvant (LifeTechnologies). They were boosted three times i.p. with 25 μg of α1β1 emulsified with incomplete Freunds's adjuvant (LifeTechnologies). The mouse with the highest anti-α1-I domain titer was boosted i.p. with 100 μg of α1β1 three days prior to fusion, and intravenously with 50 μg of α1β1 one day prior to fusion. Spleen cells were fused with FL653 myeloma cells at a 1:6 ratio and were plated at 100,000 and 33,000 per well into 96 well tissue culture plates.

Supernatants were assessed for binding to the α1β1 integrin by single color FACS. Prior to FACS analysis, supernatants were incubated with untransfected K562 cells to eliminate IgG that bound solely to the β subunit. Subsequently, 3-5 X $10^4$ K562 cells transfected with the α1 integrin subunit (K562-α1) suspended in FACS buffer (1% fetal calf serum (FCS) in PBS containing 0.5% $NaN_3$) were incubated with supernatant for 45 minutes at 4° C, washed and incubated with anti-mouse IgG conjugated to phycoerythrin. After washing twice with FACS buffer, cells were analyzed in a Becton Dickinson Flow Cytometer.

Supernantants from the resulting hybridomas were screened for binding to the α1-I domain. Briefly, 50 μl of 30 μg/ml human α1-I domain-GST fusion in PBS was coated onto wells of a 96 –well plate (Nunc) overnight at 4° C. The plates were washed with PBS, blocked with 1% BSA in PBS and the hybridoma supernatant was incubated with the I domain at room temperature for 1 hour. After extensive washing with PBS containing 0.03% Tween 20, alkaline phosphatase linked anti-mouse IgG (Jackson ImmunoResearch) was added for an additional hour. After a final wash, 1 mg/ml *p*-nitrophenylphosphate (*p*NPP) in 0.1 M glycine, 1 mM $ZnCl_2$, and 1 mM $MgCl_2$ was added for 30 minutes at room temperature, and the plates were read at O.D. 405.

Selected supernatants were tested for their ability to inhibit K562-α1 dependent adhesion to Collagen IV. K562-α1 cells were labeled with 2 mM 2',7' (bis-2-carboxyethyl-5 and 6) carboxyfluorescein penta acetoxymethylester (BCECF; Molecular Probes) in DMEM containing 0.25% BSA at 37° C for 30 minutes. Labeled cells were washed with binding buffer (10 mM Hepes, pH 7.4; 0.9% NaCl; and 2% glucose) and resuspended in binding buffer plus 5 mM $MgCl_2$ at a final concentration of 1 X $10^6$ cells/ml. 50 µl of supernatant was incubated with an equal volume of 2 X $10^5$ K562-α1 cells in wells of a 96 well plate. The plate was then centrifuged and the supernatants removed. Cells were resuspended in binding buffer and transferred to wells of a collagen-coated plate and incubated for 1 hour at 37° C. Following incubation, the non-adherent cells were removed by washing three times with binding buffer. Attached cells were analyzed on a Cytofluor (Millipore).

We initially identified 19 hybridomas, the supernatants of which bound to human leukemia K562 cells expressing the α1β1 integrin (K562-α1) and to the α1-I domain. The immunoglobulins were purified from each of these hybridomas and tested for the ability to block either K562-α1 or α1- I domain binding to collagen IV. The mAbs fall into two classes: those that block and those that do not block α1β1 function. For example, while the mAbs produced by clones AEF3, BGC5, AQC2 and AJH10 bind the α1-I domain (Fig. 13A, data not shown for BGC5), only mAbs AJH10 and AQC2 inhibit α1-I domain-dependent (Fig. 13B; Fig. 16B) or K562-α1 (Fig. 13C; Fig. 16C) adhesion to collagen IV.

Sequencing of the Complementarity Determining Regions. To establish the clonal origin of this panel of mAbs, we amplified by PCR and sequenced the CDRs from 12 of the 19 antibodies (data not shown).

2 µg of mRNA, isolated from $10^7$ hybridomas ( FastTrack mRNA isolation kit , Invitrogen), was reverse transcribed (Ready-To-Go You Prime First Strand Kit, Pharmacia Biotech) using 25 pM each of the following primers: heavy chain VH1FOR-2 (Michishita et al., 1993, *Cell* 72:857-867); light chain, VK4FOR, which defines four separate oligos (Kern et al., 1994, *J. Biol. Chem.* 269:22811-22816). For each hybridoma, heavy and light chains were amplified in four separate PCR reactions using various combination of the following oligos: 1) Heavy chain:

VH1FR1K (Kamata et al., 1995, *J. of Biol. Chem.* 270:12531-12535), VH1BACK, VH1BACK (Baldwin et al.(1998) *Structure* 6, 923-935), $V_H$fr1a, $V_H$fr1b, $V_H$fr1e, $V_H$fr1f, $V_H$fr1g (Ignatius et al. (1990) *J. Cell Biol.* 111, 709-720), or VH1FOR-2 (Michishita, M., Videm, V., and Arnaout, M. A. (1993) *Cell* 72, 857-867); 2) Light chain: VK1BACK (Baldwin et al. (1998) *Structure* 6, 923-935), VK4FOR, VK2BACK oligos (Kern et al. (1994) *J. Biol. Chem.* 269, 22811-22816), or $V_K$fr1a, $V_H$fr1c, $V_H$fr1e, $V_H$fr1f (Ignatius et al. (1990) *J. Cell Biol.* 111, 709-720). Products were amplified (5 min at 95° C, 50 cycles of 1 min at 94° C, 2 min at 55° C, 2 min at 72° C, and a final cycle of 10 min at 72° C), gel purified (QIAquick, Qiagen), and sequenced directly using various of the listed oligos on an ABI 377 Sequencer.

Sequences from clones producing function-blocking mAbs were nearly identical across all the complementarity-determining regions (CDRs) and the intervening framework regions suggesting that these hybridomas are clonally related.

**Example 16**

*Immunoblotting and FACS Analysis*. Sequences of the variable regions of the non-blocking antibodies were markedly different from the clonally related family of sequences found for the blocking antibodies. As the blocking antibodies appear to originate from a single clone, we chose two (AJH10 and AQC2) to characterize further.

Immunoblotting The smooth muscle cell layer dissected from sheep aorta, and K562-α1 cells were extracted with 1% Triton X-100 in 50 mM Hepes, pH 7.5, 150 mM NaCl, 10 mM phenylmethylsulfonyl flouride (PMSF), 20 μg/ml aprotinin, 10 μg/ml leupeptin, 10 mM ethylenediaminetetraacetic acid (EDTA). Samples were subjected to 4-20% gradient SDS-PAGE, and electroblotted onto nitrocellulose membranes. The blots were blocked with 5% dry milk in TBS; washed in TBS containing 0.03% Tween-20, and incubated with antibodies in blocking buffer containing 0.05% $NaN_3$ for 2 hours. Blots were then washed as before, incubated with horseradish peroxidase conjugated anti-mouse IgG for one hour, washed again and then treated with ECL reagent (Amersham). Blots were then exposed to film (Kodak) for 30 to 60 seconds, and developed.

Immunoblotting and FACS analysis (Fig. 14) demonstrate that AJH10 reacts with human, rabbit, and sheep, but not rat $\alpha 1\beta 1$ integrin suggesting that the blocking mAbs bind to an evolutionarily conserved, linear epitope. The non-blocking mAbs were neither efficient at immunoblotting nor did they react with species other than human.

**Example 17**

*Binding of the α1- I domain to collagen is divalent cation-dependent*

*A. Purification of the α1- I domains.*

The α1-I domains were expressed in *E. coli* as GST (glutathione-S-transferase) fusion proteins containing a thrombin cleavage site at the junction of the sequences. The clarified supernatant from cells lysed in PBS was loaded onto a glutathione Sepharose 4B column (Pharmacia) which was washed extensively with PBS. The α1-I domain-GST fusion protein was eluted with 50 mM Tris-HCl, pH 8.0, 5 mM glutathione (reduced). For denaturation studies, the I domain was cleaved with thrombin in 50 mM Tris, pH 7.5, and purified from the GST fusion partner. DTT was added to 2 mM and the sample was loaded on a glutathione Sepharose 4B column. The flow-through and wash fractions were pooled and loaded onto a Q Sepharose FF column (Pharmacia). The α1-I domain was eluted with 50 mM Tris HCl, pH 7.5, 10 mM 2-mercaptoethanol, 75 mM NaCl. The purified I domain displayed its predicted mass (Lee et al. (1995) *Structure* 3, 1333-1340, 871 Da) by electrospray ionization-mass spectrometry (ESI-MS), migrated as a single band by SDS-PAGE, and the protein eluted as a single peak of appropriate size by size exclusion chromotography on a Superose 6 FPLC column (Pharmacia).

*B. Functional Analysis*

96 well plates were coated overnight at 4° C with 1 μg/ml collagen IV (Sigma) or collagen Type I (Collaborative Biomedical), washed with Triton buffer (0.1% Triton X-100; 1 mM $MnCl_2$; 25 mM Tris-HCl; 150 mM NaCl), and blocked with 3% bovine serum albumin (BSA) in 25 mM Tris-HCl; 150 mM NaCl (TBS). Serial dilutions of the α1- I domain-GST fusion protein in TBS containing 1 mM $MnCl_2$ and 3% BSA were incubated on the coated plates at room temperature for 1 hour, and washed in Triton buffer. Bound α1- I domain was detected with serial

additions of 10 μg/ml biotinylated anti-GST polyclonal antibody (Pharmacia); ExtrAvidin-horseradish peroxidase (Sigma) diluted 1:3000 in TBS containing 1 mM $MnCl_2$ and 3% BSA, and 1-Step ABTS (2,2'-Azine-di[3-ethylbenzthiazoline sulfonate]; Pierce). Plates were read at O.D. 405 on a microplate reader (Molecular Devices).

*Results.*

The human and rat (95% identity to human) α1-I domains were expressed in *E. coli* as GST-fusion proteins and purified over glutathione sepharose. Both proteins were examined for binding to collagen I and IV using a variation of an ELISA-based assay previously described (Qu, A., and Leahy, D. J. (1995) *Proc. Natl. Acad. Sci. USA* 92, 10277-10281). The human α1-I domain binds collagen IV with better efficiency than collagen I (Fig. 15A). An antibody specific to the α1-I domain, but not an antibody specific to the α2-I domain (Fig. 15B) abrogated binding to both ligands (data for collagen I is not shown). Both $Mn^{2+}$ and $Mg^{2+}$ stimulated binding, and EDTA reduced binding to background levels (Fig. 15C). No measurable differences in ligand binding were detected between the human and rat α1-I domains suggesting that the sequence differences between species are not functionally relevant (data not shown). Thus, the α1-I domain, specifically, require cation for efficient ligand binding.

**Example 18**

*A Cation-Dependent Epitope Resides near the MIDAS motif.* We exploited the observation that AJH10 recognizes the human, but not the rat α1-I domain sequences to map the epitope for the α1β1 function-blocking mAbs. The human and rat sequences differ by only 12 amino acids, 4 of which lie in a stretch of 6 amino acids (aa 92-97, Fig. 11A) adjacent to the critical threonine (Fig. 11A, aa 98) within the MIDAS motif. To test the hypothesis that the 6 amino acid residues, Val-Gln-Arg-Gly-Gly-Arg, comprise the epitope for the blocking mAbs, we constructed a chimeric I domain (RΔH), exchanging the rat residues G92, R93, Q94, and L97 for the corresponding human residues, V, Q, R, and R, respectively. AJH10, along with all the function-blocking mAbs, recognizes the chimeric I domain (RΔH; Fig. 11B).

To orient these residues with respect to the MIDAS domain in the

tertiary structure of the α1- I domain, we modeled the α1-I domain using the coordinates of the crystal structure of the α2 I domain.

A homology model of the human α1 I –domain was built using the X-ray crystal structure of the human α2 I-domain (Ward et al. (1989) *Nature* 341, 544-546). The model was built using the homology modeling module of Insight II (version 2.3.5; Biosym Technologies). The program CHARMM (Clackson et al. (1991) *Nature* 352, 624-628) was used with the all-hydrogen parameter set 22 with a distant dependent dielectric constant of two times the atom separation distance. We first did 1000 steps of steepest descent minimization with mass-weighted harmonic positional constraints of 1kcal/(mol Å$^2$) on all atoms of the α1-I domain. This minimization was followed by another 1000 steps of steepest descent and 5000 steps of Adopted-Basis Newton Raphson with constraints of 0.1 kcal/( mol Å$^2$) on the C-α atoms of the α1-I domain to avoid significant deviations from the α2-I domain X-ray crystal structure.

The α1β1 and α2β1 integrin sequences exhibit 51% identity with no insertions or deletions, suggesting that the overall structure of the two I domains will be similar. The metal coordination site is predicted to be the same in the α1-I domain as in the α2-I domain, and the residues that comprise the epitope for the blocking mAbs lie on a loop between helix α3 and helix α4 which contains the threonine within the MIDAS motif critical for cation binding. The α1-I domain model predicts that the amide nitrogen of Q92 (Fig. 11A) hydrogen bonds with the carbonyl group of I33, the residue adjacent to S32. Thus, the loop that contains the epitope may play a functional role in stabilizing the MIDAS region.

**Example 19**

Monoclonal antibody AQC2 (i.e., mAQC2; "m" for murine) (Example 15, *supra*) is an $IgG_1$, kappa antibody. To identify the nucleotide sequences encoding the heavy and light chains of this antibody, total cellular RNA from AQC2 murine hybridoma cells was obtained by using a QIAGEN RNEASY midi kit in accordance with the manufacturer's instructions. Then cDNAs encoding the variable regions of the heavy and light chains were cloned by RT-PCR from total cellular RNA using a GIBCO BRL SUPERSCRIPT Preamplification System for First Strand cDNA

Synthesis following the manufacturer's recommended protocol. Random hexamers were used for priming.

The heavy chain variable domain of mAQC2 was amplified by PCR from the first strand cDNA with the primers: 5' TGA GGA GAC GGT GAC CGT GGC CCT TGG CCC C 3' (SEQ ID NO:11) and 5' AGG TSM ARC TGC AGS AGT CWG G 3' (S=C/G, M=A/C, R=A/G, and W=A/T) (SEQ ID NO:12). The PCR was subjected to 30 cycles using Clontech's Advantage Taq polymerase: denature 30 sec at 94°C, anneal 1 min at 50°C, and elongate 1.5 min at 68°C. The mAQC2 light chain with its signal sequence was amplified by PCR using the primers: 5' ACT AGT CGA CAT GGA TTT WCA GGT GCA GAT TWT CAG CTT C 3' (W=A/T) (SEQ ID NO:13) and 5' ACT GGA TGG TGG GAA GAT GGA 3' (SEQ ID NO:14). The PCR was subjected to 30 cycles using Stratagene's cloned Pfu polymerase: denature 1 min at 94°C, anneal 1 min at 50°C, and elongate 2 min at 72°C. The PCR products for the heavy and light chains were gel-purified using a QIAGEN QIAQUICK gel extraction kit following the manufacturer's recommended protocol.

Purified heavy chain product was subcloned into Invitrogen's pCR2.1-TOPO TA vector using its TOPO TA cloning kit. Purified light chain was subcloned into Invitrogen's pCRbluntIITOPO vector using its Zero blunt TOPO cloning kit following the manufacturer's recommended protocol. Inserts from multiple independent subclones were sequenced. With the exception of degenerate positions within the PCR primers, the insert sequences of the independent subclones were identical.

The polypeptide sequences of mAQC2 were deduced from their coding sequences. The N-terminal amino acid sequence for the mature light chain predicted by the cDNA sequence from the PCR product amplified with a signal sequence exactly matched the N-terminal sequence of purified mAQC2 light chain derived from Edman degradation (DVKVVESGG; SEQ ID NO:15). BLAST analyses of the variable domain sequences confirmed their immunoglobulin identity.

The polypeptide sequence of the light chain variable domain of mAQC2 is shown below:

1 QIVLTQFPAL MSASPGEKVT MTCSASSSVN HMFWYQQKPK
41 SSPKPWIYLT **SNLASGVPAR** FSGSGSGTSY SLTISSMEAE
81 DAATYYCQQW **SGNPWTFGGG** TKLEIK 106
(SEQ ID NO:1)

The CDRs are shown in boldface. The CDRs are defined according to Kabat et al., Sequences of Proteins of Immunological Interest, 5th Edition, The United States Department of Health and Human Services, The United States Government Printing Office, 1991. Using the Kabat numbering system, SEQ ID NO:1 is represented as follows, where a dash denotes the absence of an amino acid:

1 QIVLTQFPAL MSASPGEKVT MTCSASS-SV NHMFWYQQKP
41 KSSPKPWIYL **TSNLASGVPA** RFSGSGSGTS YSLTISSMEA
81 EDAATYYCQQ **WSGNPWTFGG** GTKLEIK 107

The polypeptide sequence of the heavy chain variable domain of mAQC2 is:

1 DVKVVESGGG LVKPGGSLKL ACAASGFSFS RYTMSWVRQI
41 PEKRLEWVAT **ISGGGHTYYL** DSVKGRFTIS RDNAKNTLYL
81 QMSSLRSEDT AMYYCTRGFG DGGYFDVWGQ GTTVTVSS
(SEQ ID NO:2)

The CDRs are shown in boldface. Using the Kabat numbering system, SEQ ID NO:2 is represented as follows, where positions numbers are consecutive numerals unless otherwise indicated:

1 DVKVVESGGG LVKPGGSLKL ACAASGFSFS RYTMSWVRQI
41 PEKRLEWVAT **ISGGGHTYYL** DSVKGRFTIS RDNAKNTLYL
81 QM
82a-c SSL
83 RSEDTAMY YCTRGFGDGG

| | | | |
|---|---|---|---|
| 100a-b | YF | | |
| 101 | DVWGQGTTVT | VSS | 113 |

As used herein, residue position numbers of variable domains are designated in accordance with the Kabat numbering system unless otherwise indicated.

**Example 20**

This example describes the generation of a murine-human chimeric antibody, chAQC2.

The cDNAs encoding the variable regions of the mAQC2 heavy and light chains were used to construct chAQC2 expression vectors, in which the mAQC2 variable regions were linked to human $IgG_1$ and kappa constant regions.

The heavy chain chimera was constructed as follows. A 0.33 kb PstI-BstEII fragment from the mAQC2 heavy chain plasmid pAND083 was subcloned into the phosphatased 2.82 kb PstI-BstEII vector fragment from the 5a8 heavy chain plasmid pLCB7, so as to add a murine heavy chain signal-encoding sequence and a murine splice donor site to the cDNA of the mAQC2 heavy chain variable region. 5a8 is a molecularly cloned CD4-specific mAb (see, e.g., Boon et al., 2002, *Toxicology* 172:191-203). In the mature heavy chain encoded by the resultant plasmid (pAND092), the N-terminus differed by five residues from the N-terminus (DVKVVE; SEQ ID NO:16) of the cognate mAQC2 heavy chain.

To correct the heavy chain N-terminus, pAND092 was subjected to unique site elimination (USE) mutagenesis using an USE mutagenesis kit (Amersham Pharmacia Biotech) following the manufacturer's recommended protocol. The Q1D, Q3K, L4V, Q5V, Q6E substitutions were encoded by the mutagenic primer 5' GCA CCA GGT GCC CAC TCC GAC GTC AAG GTG GTG GAG TCA GGG GGA GGC TTA GTG 3' (SEQ ID NO:17). Mutated plasmid clones were identified by their new AatII and HinfI sites and eliminated PstI site. The heavy chain coding sequence was then confirmed by DNA sequencing. The correctly mutated plasmid was called pAND094. The 0.43 kb NotI-HindIII fragment from pAND094 and the 1.21 kb HindIII-NotI fragment from the plasmid pEAG964 (containing a coding sequence for

a human $IgG_1$ constant region) were subcloned into the NotI site of pCH269, a plasmid derived from the pCEP4 EBV expression vector (Invitrogen). The resultant plasmid was named pAND099.

The light chain chimera was generated as follows. A 0.46 kb EcoRI fragment from the mAQC2 light chain variable domain plasmid pAND081 was subcloned into the phosphatased 2.7 kb vector fragment of the pUC-derived pNN09 cloning vector, to add a 5' NotI site. The resulting plasmid, pAND091, was subjected to mutagenesis using the Amersham USE kit (*supra*) to introduce a BglII site at the 3' end of the coding sequence. The mutagenic primer had the sequence 5' GGA GGC ACC AAG CTG GAG ATC TAA CGG GCT GAT GCT GC 3' (SEQ ID NO:18). The correctly mutated plasmid was identified by its BglII and BstYI site changes. The light chain coding sequence in the resultant plasmid pAND093 was confirmed by DNA sequencing. Then the 0.44 kb NotI-BglII light chain variable domain fragment from pAND093 and the 0.68 kb BclI-NotI fragment from the plasmid pEAG963 (containing a coding sequence for a human kappa light chain constant domain) were subcloned into the NotI site of pCH269 (*supra*), producing plasmid pAND102. To create an unblocked kappa light chain (Q1E), pAND093 was subjected to USE mutagenesis with the mutagenic primer 5' CAT AAT GTC CAG GGG AGA AAT TGT TCT CAC CCA G 3' (SEQ ID NO:19), to introduce an XmnI site. The mutated plasmid was identified by screening for an XmnI site change. The light chain sequence in the resultant plasmid pAND097 was confirmed by DNA sequencing. The 0.44 kb NotI-BglII light chain variable domain fragment from pAND097 and the 0.68 kb BclI-NotI fragment from the plasmid pEAG963 (containing a human kappa light chain constant domain) were subcloned into the NotI site of pCH269, producing plasmid pAND098.

To generate chAQC2 antibodies, expression vectors (chAQC2 heavy chain vector pAND099 + chAQC2 light chain vector pAND102, and chAQC2 heavy chain vector pAND099 + chAQC2 unblocked light chain vector pAND098) were co-transfected into 293-EBNA cells. The transfectants were tested for antibody secretion and specificity. The controls were cells transfected with the corresponding vectors without an insert or with DNA constructs encoding ch5c8 (a molecularly

cloned CD154-specific mAb described in, e.g., Elster et al., 2001, *Transplantation* 72:1473-1478) or chCBE11 (a molecularly cloned LTβR-specific mAb described in, e.g., Browning et al., 1996, *J. Biol. Chem.* 271:24934-24938).

Then transfectants with the desired antibody secretion were lysed, and protein A immunoprecipitation was performed on the lysates and conditioned medium. Western blot analysis of the precipitates performed with anti-human heavy and light chain antibodies indicated that chAQC2-transfected cells synthesized and efficiently secreted heavy and light chains at levels similar to ch5c8-transfected and chCBE11-transfected cells. Further, huVLA-1-expressing K562α1 cells were stained with the conditioned medium from the transfected cells, and FACS analysis was performed on the stained cells. The results indicated that the chAQC2 antibody produced staining patterns similar to those of mAQC2, while conditioned media from mock-transfected and ch5c8-transfected cells failed to stain K562α1 cells. Chimeric AQC2 produced from scaled-up transient transfection was purified and shown to bind to VLA-1 by FACS titration. Chimeric AQC2 with either a wildtype or a genetically unblocked light chain bound to VLA-1. See also Figs. 16A-D (discussed below).

**Example 21**

This example describes a method of humanizing the mAQC2 monoclonal antibody.

*Analysis of the mAQC2 variable domains.* The variable domains in the light and heavy chains of mAQC2 were compared with the consensus sequences for mouse and human subgroups (Kabat et al, *supra*) using the software program FASTA. The light chain variable domain was found to be a member of mouse subgroup VI with 89% identity in a 109 amino acid overlap. This domain also corresponded to human subgroup I with 72% identity in a 113 amino acid overlap. The heavy chain variable domain was found to be a member of mouse subgroup IIId with 86% identity in a 129 amino acid overlap. This heavy chain variable domain also corresponded to human subgroup III with 79% identity in a 130 amino acid overlap.

The CDRs were categorized into canonical classes according to Chothia et al., *Nature* 342, pp. 877-883 (1989). The key residues defining each

canonical class determine to a large extent the structural conformation of the CDR loop, and thus should be retained in the reshaped antibody. The L1 loop of mAQC2 fell into canonical class 1 (10 residue loop), L2 into class 1 (7 residue loop) and L3 into class 1 (9 residue loop). The H1 loop fell into class 1 (5 residue loop) and the H2 loop into class 1 (16 residue loop) residues. The H3 loop did not seem to belong to any canonical class. The canonical residues important for these classes were all included in the humanized antibodies.

Unusual framework residues in mAQC2 were determined by analyzing all mouse and human variable chain sequences in the September 1999 version of the Kabat database. It was believed that mAQC2-specific differences might indicate somatic mutations that enhance binding affinity if these differences were close to the binding site. Unusual mAQC2 residues further away from the binding site and unusual human framework residues were removed in case they would create immunogenic epitopes in the humanized antibody. Unusual framework residues found in mAQC2 were 7(F), 10(L), and 41(K) in the light chain; and 4(V), 21(A), and 40(I) in the heavy chain. None of these unusual mouse framework residues were retained the humanized antibodies.

*Modeling the structure of the variable regions*. The light and heavy chains of mAQC2 were aligned against a nonredundant database to determine which structural frames to use to construct three-dimensional models of the mAQC2 light and heavy chains. Using FASTA, the light chain was found to have 82% sequence identity to monoclonal murine antibody ab57 (1CLOL), whereas the heavy chain was found to have 76% sequence identity to murine 6d9 Fab fragment (1HYY). Using the molecular modeling software package SYBYL (Tripos Inc.), the approximate three-dimensional structures of the mAQC2 light and heavy chains were built using the light chain of ab57 and the heavy chain of 6d9, respectively. The structural integrity of the models was assessed at the console and was found to be reasonable.

*Design of the reshaped variable regions*. Two approaches were used to choose human acceptor frameworks to "accept" mAQC2's CDRs. The first approach was by homology matching and the other by using consensus human Ig sequences. Under the homology approach, the Kabat database, the nonredundant

database from NCBI, ENTREZ (The National Institutes of Health), and the Incyte database were searched using the software programs FASTA and BLAST. The choice of human acceptor frameworks was made based on sequence identity between mAQC2 frameworks and human frameworks (excluding frameworks from previously humanized antibodies) and the source of the antibody.

The frameworks from an immunoglobulin variable region gene having a GENBANK accession number of gi:587330 (human kappa subgroup I Vκ-lc147) were eventually chosen for the light chain of the humanized antibody (Welschof et al., *J. Immunol. Meth.* 179:203-14 (1995)). The frameworks from Amulc11 (Kabat ID 044469; human subgroup III) were chosen for the heavy chain of the humanized antibody (Huang et al., *J. Immunol.* 151:5290-300 (1993)).

*Back mutations of the human frameworks.* Strategies for determining which back mutations to make are available on the Humanization bY Design web sites under mirrored urls: http://mathbio.nimr.mrc.ac.uk/jsaldan and http://www.cryst.bbk.ac.uk/~ubcg07s. Previous experiments have shown that it is important to retain canonical residues, interface packing residues and unusual murine residues that are close to the binding site. In addition, residues in the "Vernier Zone," which forms a platform on which the CDRs rest (Foote et al., *J. Mol. Biol.* 224, p. 487 (1992)) and those close to CDR H3 should be considered.

Four reshaped versions were designed for each of the variable light and heavy chains, as shown in Table 1. Two of the four versions for each chain were designed by homology matching (designated huAQC2-h1 and -h2) and the other two versions by consensus matching (huAQC2-c1 and -c2). It should be noted that the sequences for huAQC-h1 heavy chain and huAQC-c1 heavy chain are identical.

**Table 1. Sequences of mAQC2, huAQC2, and human frameworks**

LIGHT CHAIN

| | FR1 | CDR1 | FR2 | CDR2 | FR3 | CDR3 | FR4 | Framework changes |
|---|---|---|---|---|---|---|---|---|
| Vk-1c147 | D--M--S-SSL---V-DR--I--* | R--Q-ISYLN | ------GKA--LL-- | AA-S-Q- | ---S---------DFT-----LQP--F----- | --SYST-L- | ------V--- | 25 |
| huAQC2-h2 | ------S-SSL---V-DR--I-- | ---------- | ------GKA--LL-- | ------- | ---S---------D-T-----LQP--F----- | --------- | ------V--- | 21 |
| huAQC2-h1 | ------S-SSL---V-DR--I-- | ---------- | ------GKA------ | ------- | ---S---------D-T-----LQP--F----- | --------- | ------V--- | 19 |
| mAQC2 | QIVLTQFPALMSASPGEKVTMTC | SASSSVNHMF | WYQQKPKSSPKPWIY | LTSNLAS | GVPARFSGSGSGTSYSLTISSMEAEDAATYYC | QQWSGNPWT | FGGGTKLEIK** | 0 |
| huAQC2-c1 | --Q---S-SSL---V-DR--I-- | ---------- | ------GKA------ | ------- | ---S---------D-T-----LQP--F----- | --------- | --Q---V--- | 21 |
| huAQC2-c2 | --Q---S-SSL---V-DR--I-- | ---------- | ------GKA--LL-- | ------- | ---S---------D-T-----LQP--F----- | --------- | --Q---V--- | 23 |

HEAVY CHAIN:

| | | FR1 | CDR1 |
|---|---|---|---|
| | AMU1C11 | E-QL-------IQ-----R-S------TV- | SNY-- |
| | huAQC2-h2 | E-QL-------IQ-----R-S------T-- | ----- |
| 5 | huAQC2-h1 | --QL--------Q-----R-S--------- | ----- |
| | mAQC2 | DVKVVESGGGLVKPGGSLKLACAASGFSFS | RYTMS |
| | huAQC2-c1 | --QL--------Q-----R-S--------- | ----- |
| | huAQC2-c2 | E-QL--------Q-----R-S------T-- | ----- |

| | | FR2 | CDR2 |
|---|---|---|---|
| 10 | AMU1C11 | ----A-G-G----S | V-YS--S---A----- |
| | huAQC2-h2 | ----A-G-G----- | ---------- |
| | huAQC2-h1 | ----A-G-G----- | ---------- |
| | mAQC2 | WVRQIPEKRLEWVA | TISGGGHTYYLDSVKG |
| | huAQC2-c1 | ----A-G-G----- | ---------- |
| 15 | huAQC2-c2 | ----A-G-G----- | ---------- |

| | | FR3 | CDR3 |
|---|---|---|---|
| | AMU1C11 | --------S---------N---A----V---AS | IRFLEWS--Y |
| | huAQC2-h2 | --------S---------N---A----V----- | ---------- |
| | huAQC2-h1 | --------S---------N---A----V----- | ---------- |
| 20 | mAQC2 | RFTISRDNAKNTLYLQMSSLRSEDTAMYYCTR | GFGDGGYFDV |
| | huAQC2-c1 | --------S---------N---A----V----- | ---------- |
| | huAQC2-c2 | --------S---------N---A----V----- | ---------- |

| | | FR4 | Framework changes |
|---|---|---|---|
| 25 | AMU1C11 | -----L----- | 20 |
| | huAQC2-h2 | -----L----- | 16 |
| | huAQC2-h1 | -----L----- | 13 |
| | mAQC2 | WGQGTTVTVSS*** | 0 |
| | huAQC2-c1 | -----L----- | 13 |
| 30 | huAQC2-c2 | -----L----- | 15 |

*Dashes indicate identity with the mAQC2 amino acid sequence.
**Part of SEQ ID NO:1.
***Part of SEQ ID NO:2.

Some of the back mutations are discussed below.

35 (1) light chain:

1 D->Q This mutation was made in all versions since previous reshaping experiments (e.g. Kolbinger et al, *Protein Eng.* 6, p. 971 (1993)) suggested its importance for antigen binding.

4 M->L This is a vernier residue and was retained in all versions.

40 46 L->P This residue is both an interfacial and vernier residue and was retained only in h1 and c1.

47 L->W This is a vernier residue and was retained only in h1 and c1.

71 F->Y This residue is in an important canonical position and was retained

in all versions.

(2) heavy chain:

1 E->D This back mutation was made in h1 (i.e., c1) only.

12 I->V The residue I is unusual in human and was retained in the h2 only.

28 T->S This is a vernier residue and was retained in h1 only.

29 V->F This is a canonical residue and was retained in all versions.

49 S->A This is a vernier residue and was retained in all versions.

93 A->T This is a vernier residue and interfacial and was retained in all versions.

94 S->R This is a canonical residue and was retained in both versions.

The huAQC2 variable regions were made by USE mutagenesis as described above, using the chAQC2 variable domain plasmids as starting templates. The human acceptor framework ("FR") cDNA sequences were Kabat #Z37334 for the light chain and Kabat #U00490 for the heavy chain. To facilitate identification of mutated plasmids, silent mutations were introduced to change restriction sites. Mutated plasmids were identified by the restriction site changes. The variable region cDNA sequences in the resultant plasmids were confirmed by DNA sequencing.

The h1 and c1 versions of heavy chain (which were identical) were made by using plasmid pAND094 as template. The mutagenic primers were: FR1 primer 5'GGT GCC CAC TCC GAC GTC CAG CTG GTC GAG TCA GGG GGA GGC TTA GTC CAG CCT GGA GGG TCC CTG AGA CTC TCC TGT GCA GCC TCT GGA TTC 3' (SEQ ID NO:20), which introduced TaqI and PvuII sites, and eliminated a DdeI site; FR2 primer 5' ATG TCT TGG GTT CGC CAG GCT CCG GGG AAG GGG CTG GAG TGG GTC GCA ACC 3' (SEQ ID NO:21), which introduced a NciI site, and eliminated BspEI and EarI sites; FR3 primer 5' TTC ACC ATC TCC AGA GAC AAT TCC AAG AAC ACC CTG TAC CTG CAG ATG AAC AGT CTG AGG GCC GAG GAC ACA GCC GTG TAT TAC TGT ACA AGA 3' (SEQ ID NO:22), which introduced PstI and DdeI sites; and FR4 primer 5' TGG GGC CAA GGT ACC CTG GTC ACC GTC TCC TCA GGT GAG 3' (SEQ ID NO:23),

which introduced KpnI and Eco0109I sites. The resultant h1 (i.e., c1) heavy chain plasmid was designated pAND104.

The c2 version of heavy chain were made by using pAND104 as template with the following mutagenic primers: FR1 primer 5' TCC TGT GCA GCC TCT GGA TTC ACC TTC AGT AGG TAT ACT ATG TCT TGG GTT 3' (SEQ ID NO:24), which introduced an AccI site; and FR1 primer 5' GCA CCA GGT GCG CAC TCC GAG GTC CAG CTG GTC GAG TCA 3' (SEQ ID NO:25), which introduced an FspI site and eliminated an AatII site. The resultant c2 heavy chain plasmid was designated pAND115.

The h2 version of heavy chain were made by using pAND115 as template with the following primer: FR1 primer 5' GAG TCA GGG GGA GGC TTA ATC CAG CCT GGA GGG TCC CTG 3' (SEQ ID NO:26), which eliminated a DdeI site. The resultant h2 heavy chain plasmid was designated pAND113.

To generate expression vectors for the huAQC2 heavy chains, the 0.43 kb NotI-HindIII heavy chain variable domain fragment from pAND104, pAND115, or pAND113, and the 1.21 kb HindIII-NotI fragment from pEAG964 (*supra*) were subcloned into the NotI site of pCH269 (*supra*). The resultant heavy chain expression plasmids were designated pAND114 (h1), pAND121 (c2), and pAND124 (h2), respectively.

The h1 version of light chain were made by using plasmid pAND093 as template. The mutagenic primers were: FR1 primer 5' CAA ATT GTT CTC ACC CAG TCT CCA TCC TCC CTG TCT GCG TCT GTA GGG GAC AGA GTC ACC ATC ACA TGC AGT GCC AGC TCA 3' (SEQ ID NO:27), which removed BstEII and PstI sites; FR2 primer 5' TTC TGG TAT CAG CAG AAG CCC GGG AAA GCC CCC AAA CCC TGG ATT 3' (SEQ ID NO:28), which introduced an NciI site; FR3 primer 5' GCT TCT GGA GTC CCT TCA CGC TTC AGT GGC AGT GGG TCT GGG ACA GAT TAC ACT CTC ACA ATC AGC AGC CTG CAA CCT GAA GAT TTT GCC ACT TAT TAC TGC CAG 3' (SEQ ID NO:29), which introduced a DdeI site and eliminated EcoO109I and AvaII sites; and FR4 primer 5' GGT GGA GGC ACT AAG GTG GAG ATC TAA CGG GCT 3' (SEQ ID NO:30), which introduced DdeI and StyI sites. The resultant h1 light chain plasmid was designated pAND103.

The h2 version of light chain were made by using pAND103 as template with the following primer: FR2 primer 5' CCC GGG AAA GCG CCC AAA CTC CTG ATT TAT CTC ACA TCC 3' (SEQ ID NO:31), which introduced HhaI and HaeII sites. The resultant h2 light chain plasmid was designated pAND116.

The c1 version of light chain used plasmid pAND103 template with the following primers: FR1 primer 5' GCC TCA GTC ATA ATG TCC CGG GGA CAA ATT CAG CTC ACC CAG TCT CCA TCC 3' (SEQ ID NO:32), which introduced SmaI, NciI, and HpaII sites; FR4 primer 5' GGT AAC CCG TGG ACG TTC GGT CAG GGC ACT AAG GTG GAG ATC TAA CGG GCT 3' (SEQ ID NO:33), which introduced a Bsp1286I site. The resultant c1 light chain plasmid was designated pAND118.

The c2 version of light chain were made by using plasmid pAND116 template with the following primers: FR1 primer 5' GCC TCA GTC ATA ATG TCC CGG GGA CAA ATT CAG CTC ACC CAG TCT CCA TCC 3' (SEQ ID NO:34), which introduced SmaI, NciI, and HpaII sites; FR4 primer 5' GGT AAC CCG TGG ACG TTC GGT CAG GGC ACT AAG GTG GAG ATC TAA CGG GCT 3' (SEQ ID NO:35), which introduced a Bsp1286I site. The resultant c2 light chain plasmid was designated pAND119.

To generate expression vectors for the huAQC2 light chains, the 0.44 kb NotI-BglII light chain variable domain fragment from pAND103, pAND116, pAND118, or pAND119, and the 0.68 kb BclI-NotI fragment from pEAG963 (*supra*) were subcloned into the NotI site of pCH269 (*supra*). The resultant light chain expression vectors were designated pAND117 (h1), pAND120 (h2), pAND122 (c1), and pAND123 (c2), respectively.

The expression vectors were co-transfected into 293-EBNA cells, and transfected cells were tested for antibody secretion and specificity. Cells transfected with an empty vector served as negative control. The whole cell lysates and the conditioned medium were immuno-precipitated with protein A. Western blot analysis of the precipitates (developed with anti-human heavy and light chain antibodies) indicated that huAQC2-transfected cells synthesized and efficiently secreted heavy and light chains at levels similar to chAQC2-transfected cells.

FACS analysis of VLA-1-expressing K562α1 cells stained with conditioned medium from the transfected cells was then performed. To do so, the K562α1 cells were incubated with the conditioned medium on ice for 120 min. The cells were then washed three times with a FACS buffer (PBS with 5% FBS and 0.05% sodium azide). The washed cells were resuspended in the buffer and incubated with PE-conjugated anti-human IgG (H + L) (Jackson ImmunoResearch Laboratories, Inc.) on ice for 30 min on ice. After the incubation, the cells were washed three times with the FACS buffer, and resuspended in the FACS buffer for analysis. The data are shown in Table 2, in which HuAQC2-h1 refers to an mAb consisting of the h1 version of the huAQC2 heavy chain (HC) and the h1 version of the huAQC2 light chain (LC) (see Table 1). Likewise, huAQC-h2 is an mAb consisting of the h2 versions of the heavy and light chains, huAQC2-c1 the c1 versions, and huAQC2-c2 the c2 versions. In the table, relative MFI refers to mean MFI normalized to that observed for chAQC2 blocked. Data shown represents the average from two independent transfections. These data indicated that the huAQC2-h2 and -c2 mAbs bound less well than huAQC2-h1 and -c1 relative to chAQC2.

**Table 2. FACS staining of K562α1 cells by chAQC2 and huAQC2**

| | Light chain | Heavy chain | Relative MFI |
|---|---|---|---|
| chAQC2 | pAND102 | pAND099 | 1.00 |
| huAQC2-h1 | pAND117 | pAND114 | 1.50 |
| huAQC2-h2 | pAND120 | pAND124 | 0.64 |
| huAQC2-c1 | pAND122 | pAND114 | 1.50 |
| huAQC2-c2 | pAND123 | pAND121 | 0.68 |
| huAQC2 LC c1/HC c2 | pAND122 | pAND121 | 2.21 |
| huAQC2 LC c2/HC c1 | pAND123 | pAND114 | 0.76 |
| huAQC2 LC unblocked c1/HC c2 | pAND150* | pAND121 | 0.75 |
| huAQC2 LC L46P c2/HC c2 | pAND133** | pAND121 | 1.50 |
| huAQC2 LC L47W c2/HC c2 | pAND132*** | pAND121 | 1.00 |

*It encodes huAQC2 LC c1 with an unblocked N-terminus Q1D.
**It encodes huAQC2 LC c2 with L46P.
***It encodes huAQC2 LC c2 with L47W.

Co-transfections of 293-EBNA cells with chAQC2 and huAQC2-h1, -h2, -c1 and -c2 were scaled up. Antibodies in the conditioned media were purified with Protein A-Sepharose. Purified mAbs were assayed by FACS for activity. The protocol as follows.

1. Count cells from flask that was split 1:4 on the day prior to the assay.

2. Pellet cells and resuspend at 2.5e5 cells/ml in FACS buffer (5% FBS in PBS- with 0.02% NaAzide).

3. Pipette 100 µl of cells into the wells of a 96 well V bottom plate.

4. Prepare 1:3 serial dilutions of AQC2 starting at 3 µg/ml in FACS buffer.

5. Pellet the cells for 5 minutes at 800 X g and flick plate to remove buffer.

6. Resuspend the cells in 100 µl of the diluted antibody series.

7.Incubate for 2 hours on ice.

8. Wash plate. Pellet the cells for 3 minutes at 800 X g and flick plate to remove buffer.

9. Resuspend the cells in 100 µl of secondary antibody (diluted 1:100 in FACS buffer).

10. Incubate for 30 minutes on ice.

11. Wash plate (see above).

12. Resuspend cells in 25 µl of FACS buffer.

13. Centrifuge the FACS tubes briefly to ensure that the 50 µl is in the bottom of the tubes.

14. Vortex each tube vigorously and collect 5000 events.

The data are shown in Fig. 17. These data confirmed that huAQC2-h2 and -c2 bound less well than huAQC2-h1 and -c1 relative to chAQC2.

The consensus versions of huAQC2 were studied further because they would be less immunogenic when used to treat patients with chronic indications. Mix-and-match cotransfections were performed to identify whether a single chain was responsible for the apparent decrease in binding seen with huAQC2-c2. The co-transfections suggested that the reduction could be attributed to the c2 light chain (encoded by pAND123), which differed from the c1 light chain (encoded by pAND122) at only two residues in the FR2 region: P46L and W47L.

To examine the individual contributions of each of these two changes, new c2 light chain expression vectors were constructed. Plasmid pAND125, the L47W variant of the c2 light chain was made using pAND119 as a template with the

following mutagenic primer: FR2 primer 5' GGG AAA GCA CCC AAA CTC TGG ATC TAT CTC ACA TCC AAC 3' (SEQ ID NO:36), which introduced HhaI and HaeII sites. Plasmid pAND126, the L46P variant of the c2 light chain, was made by using pAND119 as a template with the following mutagenic primer: FR2 primer 5' AAG CCC GGG AAG GCG CCC AAA CCC CTG ATT TAT CTC ACA TCC AAC 3' (SEQ ID NO:37), which introduced BsaHI, BanI, and NarI sites. Expression vectors for these new huAQC2 light chains were made by subcloning the 0.44 kb NotI-BglII light chain variable domain fragment from pAND125 or pAND126, and the 0.68 kb BclI-NotI fragment from pEAG963 (*supra*) into the NotI site of pCH269 (*supra*). The resultant plasmids were designated pAND132 (c2 with L47W), and pAND133 (c2 with L46P), respectively.

Co-transfections of the new light chain plasmids with each of the huAQC2 heavy chain plasmids were performed. VLA-1 binding was examined by FACS. The data demonstrate that the L47W back mutation failed to improve binding. The L46P mutation improved the peak of the binding curve, but the EC50 was still right-shifted relative to the behavior of huAQC2 version 1 (Table 2, *supra*). These results suggested that both back mutations were needed for full binding activity.

A genetically unblocked c1 light chain was also made, since the Q1D variant would be one residue more "humanized." The Q1D mutant, designated pAND148, was made with the template pAND118 with the following mutagenic primer: FR1 primer 5' GTC ATA ATG TCC CGG GGA GAT ATC CAG CTC ACC CAG TCT 3' (SEQ ID NO:38), which introduced a new EcoRI site and removed an ApoI site. An expression vector for this last variant of the huAQC2 light chain was made by subcloning the 0.44 kb NotI-BglII light chain variable domain fragment from pAND148 and the 0.68 kb BclI-NotI fragment from pEAG963 into the NotI site of pCH269, producing the light chain expression vector pAND150 (c1 with unblocked N-terminus Q1D). Co-expression of the genetically unblocked light chain with the c2 heavy chain (i.e., "huAQC2 LC c1 unblocked/HC c2"; designated huAQC2-c4) was equivalent to that of "huAQC2 LC c1/HC c2" (designated as huAQC2-c3). VLA-1 binding was confirmed by FACS on VLA1-expressing K562α1 cells (Table 2).

Co-transfections of 293-EBNA cells with chAQC2 and huAQC2-h1, -h2, -c1, -c2, -c3, and -c4. Antibodies in the conditioned media were purified on Protein A-Sepharose. The purified mAbs were assayed for activity (Figs. 17 and 18). HuAQC2-c3 was chosen as the drug candidate, since its properties were more similar to chAQC2. Vectors were then designed for stable expression of huAQC2-c3 in CHO cells. The vectors contained a cDNA for the huAQC2 c1 LC or c2 HC, with the 5' and 3' UTRs eliminated and the heavy chain C-terminal lysine genetically deleted to ensure product homogeneity. The final vectors were pAND162 (light chain), pAND160 (heavy chain). As used herein, huAQC2-c3 is also called hAQC2.

The full polypeptide sequences of hAQC2 are as follows.

Light Chain (Plasmid: pAND162)

1 QIQLTQSPSS LSASVGDRVT ITCSASSSVN HMFWYQQKPG KAPKPWIYLT

51 SNLASGVPSR FSGSGSGTDY TLTISSLQPE DFATYYCQQW SGNPWTFGQG

101 TKVEIKRTVA APSVFIFPPS DEQLKSGTAS VVCLLNNFYP REAKVQWKVD

151 NALQSGNSQE SVTEQDSKDS TYSLSSTLTL SKADYEKHKV YACEVTHQGL

201 SSPVTKSFNR GEC

(SEQ ID NO:3)

Heavy Chain (Plasmid: pAND160)

1 EVQLVESGGG LVQPGGSLRL SCAASGFTFS RYTMSWVRQA PGKGLEWVAT

51 ISGGGHTYYL DSVKGRFTIS RDNSKNTLYL QMNSLRAEDT AVYYCTRGFG

101 DGGYFDVWGQ GTLVTVSSAS TKGPSVFPLA PSSKSTSGGT AALGCLVKDY

151 FPEPVTVSWN SGALTSGVHT FPAVLQSSGL YSLSSVVTVP SSSLGTQTYI

201 CNVNHKPSNT KVDKKVEPKS CDKTHTCPPC PAPELLGGPS
VFLFPPKPKD
251 TLMISRTPEV TCVVVDVSHE DPEVKFNWYV DGVEVHNAKT
KPREEQYNST
301 YRVVSVLTVL HQDWLNGKEY KCKVSNKALP APIEKTISKA
KGQPREPQVY
351 TLPPSRDELT KNQVSLTCLV KGFYPSDIAV EWESNGQPEN
NYKTTPPVLD
401 SDGSFFLYSK LTVDKSRWQQ GNVFSCSVMH EALHNHYTQK SLSLSPG
(SEQ ID NO:4)

Other heavy and light chain polypeptide and nucleotide sequences are shown below.

A. chAQC2 heavy chain (Pand099) (SEQ ID NOs:39 and 40. The former No refers to the nucleotide sequence and the latter to the polypeptide sequence. The same order is used in the following numbering.)

1
GACGTCAAGGTGGTGGAGTCAGGGGGAGGCTTAGTGAAGCCTGGAGGGTCCCTGAAA
CTC
D V K V V E S G G G L V K P G G S L
K L

61
GCCTGTGCAGCCTCTGGATTCAGTTTCAGTAGATATACTATGTCTTGGGTTCGCCAG
ATT
A C A A S G F S F S R Y T M S W V R
Q I

121
CCGGAGAAGAGGCTGGAGTGGGTCGCAACCATTAGTGGTGGTGGTCACACCTACTAT
CTA

P E K R L E W V A T I S G G G H T Y
Y L

181
GACAGTGTGAAGGGCCGATTCACCATCTCCAGAGACAATGCCAAGAACACCCTGTAC
CTG
D S V K G R F T I S R D N A K N T L
Y L

241
CAAATGAGCAGTCTGAGGTCTGAGGACACAGCCATGTATTACTGTACAAGAGGTTTT
GGA
Q M S S L R S E D T A M Y Y C T R G
F G

301
GACGGGGGGTACTTCGATGTCTGGGGCCAAGGGACCACGGTCACCGTCTCCTCA
D G G Y F D V W G Q G T T V T V S S

B. hAQC2 HC h1 and c1 (pAND114) (SEQ ID NOs:41 and 42)

1
GACGTCCAGCTGGTCGAGTCAGGGGGAGGCTTAGTCCAGCCTGGAGGGTCCCTGAGA
CTC
D V Q L V E S G G G L V Q P G G S L
R L

61
TCCTGTGCAGCCTCTGGATTCAGTTTCAGTAGATATACTATGTCTTGGGTTCGCCAG
GCT
S C A A S G F S F S R Y T M S W V R
Q A

121
CCGGGGAAGGGGCTGGAGTGGGTCGCAACCATTAGTGGTGGTGGTCACACCTACTAT
CTA
P G K G L E W V A T I S G G G H T Y
Y L

181
GACAGTGTGAAGGGCCGATTCACCATCTCCAGAGACAATTCCAAGAACACCCTGTAC
CTG
D S V K G R F T I S R D N S K N T L
Y L

241
CAGATGAACAGTCTGAGGGCCGAGGACACAGCCGTGTATTACTGTACAAGAGGTTTT
GGA
Q M N S L R A E D T A V Y Y C T R G
F G

301
GACGGGGGGTACTTCGATGTCTGGGGCCAAGGTACCCTGGTCACCGTCTCCTCA
D G G Y F D V W G Q G T L V T V S S

C. hAQC2 h2 heavy chain (pAND124) (SEQ ID NOs:43 and 44)

1
GAGGTCCAGCTGGTCGAGTCAGGGGGAGGCTTAATCCAGCCTGGAGGGTCCCTGAGA
CTC
E V Q L V E S G G G L I Q P G G S L
R L

61
TCCTGTGCAGCCTCTGGATTCACCTTCAGTAGGTATACTATGTCTTGGGTTCGCCAG
GCT

S C A A S G F T F S R Y T M S W V R
Q A

121
CCGGGGAAGGGGCTGGAGTGGGTCGCAACCATTAGTGGTGGTGGTCACACCTACTAT
CTA
P G K G L E W V A T I S G G G H T Y
Y L

181
GACAGTGTGAAGGGCCGATTCACCATCTCCAGAGACAATTCCAAGAACACCCTGTAC
CTG
D S V K G R F T I S R D N S K N T L
Y L

241
CAGATGAACAGTCTGAGGGCCGAGGACACAGCCGTGTATTACTGTACAAGAGGTTTT
GGA
Q M N S L R A E D T A V Y Y C T R G
F G

301
GACGGGGGGTACTTCGATGTCTGGGGCCAAGGTACCCTGGTCACCGTCTCCTCAGG
D G G Y F D V W G Q G T L V T V S S

D. hAQC2 c2 heavy chain (pAND121) (SEQ ID NOs:45 AND 2)

1
GAGGTCCAGCTGGTCGAGTCAGGGGGAGGCTTAGTCCAGCCTGGAGGGTCCCTGAGA
CTC
E V Q L V E S G G G L V Q P G G S L
R L

61
TCCTGTGCAGCCTCTGGATTCACCTTCAGTAGGTATACTATGTCTTGGGTTCGCCAG
GCT
S C A A S G F T F S R Y T M S W V R
Q A

121
CCGGGGAAGGGGCTGGAGTGGGTCGCAACCATTAGTGGTGGTGGTCACACCTACTAT
CTA
P G K G L E W V A T I S G G G H T Y
Y L

181
GACAGTGTGAAGGGCCGATTCACCATCTCCAGAGACAATTCCAAGAACACCCTGTAC
CTG
D S V K G R F T I S R D N S K N T L
Y L

241
CAGATGAACAGTCTGAGGGCCGAGGACACAGCCGTGTATTACTGTACAAGAGGTTTT
GGA
Q M N S L R A E D T A V Y Y C T R G
F G

301
GACGGGGGGTACTTCGATGTCTGGGGCCAAGGTACCCTGGTCACCGTCTCCTCAGG
D G G Y F D V W G Q G T L V T V S S

E. chAQC2 blocked light chain (Pand102) (SEQ ID NOs:46 and 47)

```
1 CAAATTGTTCTCACCCAGTTTCCAGCACTCATGTCTGCGTCTCCAGGGGAGAAGGTCACC
  Q  I  V  L  T  Q  F  P  A  L  M  S  A  S  P  G  E  K
V T

61
ATGACCTGCAGTGCCAGCTCAAGTGTAAATCACATGTTCTGGTATCAGCAGAAGCCA
AAA
   M  T  C  S  A  S  S  S  V  N  H  M  F  W  Y  Q  Q  K
P K

121
TCCTCCCCCAAACCCTGGATTTATCTCACATCCAACCTGGCTTCTGGAGTCCCTGCT
CGC
   S  S  P  K  P  W  I  Y  L  T  S  N  L  A  S  G  V  P
A R

181
TTCAGTGGCAGTGGGTCTGGGACCTCTTACTCTCTCACAATCAGCAGCATGGAGGCT
GAA
   F  S  G  S  G  S  G  T  S  Y  S  L  T  I  S  S  M  E
A E

241
GATGCTGCCACTTATTACTGCCAGCAGTGGAGTGGTAACCCGTGGACGTTCGGTGGA
GGC
   D  A  A  T  Y  Y  C  Q  Q  W  S  G  N  P  W  T  F  G
G G
301 ACCAAGCTGGAGATCAAA
    T  K  L  E  I  K
```

F. hAQC2 h1 light chain (pAND117) (SEQ ID NOs:48 and 49)

```
 1 CAAATTGTTCTCACCCAGTCTCCATCCTCCCTGTCTGCGTCTGTAGGGGACAGAGTCACC
   Q  I  V  L  T  Q  S  P  S  S  L  S  A  S  V  G  D  R
V  T

 61
5 ATCACATGCAGTGCCAGCTCAAGTGTAAATCACATGTTCTGGTATCAGCAGAAGCCC
GGG
   I  T  C  S  A  S  S  S  V  N  H  M  F  W  Y  Q  Q  K
P  G

121
10 AAAGCCCCCAAACCCTGGATTTATCTCACATCCAACCTGGCTTCTGGAGTCCCTTCA
CGC
   K  A  P  K  P  W  I  Y  L  T  S  N  L  A  S  G  V  P
S  R

181
15 TTCAGTGGCAGTGGGTCTGGGACAGATTACACTCTCACAATCAGCAGCCTGCAACCT
GAA
   F  S  G  S  G  S  G  T  D  Y  T  L  T  I  S  S  L  Q
P  E

241
20 GATTTTGCCACTTATTACTGCCAGCAGTGGAGTGGTAACCCGTGGACGTTCGGTGGA
GGC
   D  F  A  T  Y  Y  C  Q  Q  W  S  G  N  P  W  T  F  G
G  G

301 ACTAAGGTGGAGATCAAA
25    T  K  V  E  I  K
```

G. hAQC2 h2 light chain (pAND120) (SEQ ID NOs:50 and 51)

```
  1
CAAATTGTTCTCACCCAGTCTCCATCCTCCCTGTCTGCGTCTGTAGGGGACAGAGTC
ACC
    Q  I  V  L  T  Q  S  P  S  S  L  S  A  S  V  G  D  R
5 V  T

 61
ATCACATGCAGTGCCAGCTCAAGTGTAAATCACATGTTCTGGTATCAGCAGAAGCCC
GGG
    I  T  C  S  A  S  S  S  V  N  H  M  F  W  Y  Q  Q  K
10 P  G

121
AAAGCGCCCAAACTCCTGATTTATCTCACATCCAACCTGGCTTCTGGAGTCCCTTCA
CGC
    K  A  P  K  L  L  I  Y  L  T  S  N  L  A  S  G  V  P
15 S  R

181
TTCAGTGGCAGTGGGTCTGGGACAGATTACACTCTCACAATCAGCAGCCTGCAACCT
GAA
    F  S  G  S  G  S  G  T  D  Y  T  L  T  I  S  S  L  Q
20 P  E

241
GATTTTGCCACTTATTACTGCCAGCAGTGGAGTGGTAACCCGTGGACGTTCGGTGGA
GGC
    D  F  A  T  Y  Y  C  Q  Q  W  S  G  N  P  W  T  F  G
25 G  G

301 ACTAAGGTGGAGATCAAA
    T  K  V  E  I  K
```

H. hAQC2 c1 light chain (pAND122) (SEQ ID NOs:52 and 1)

```
  1
CAAATTCAGCTCACCCAGTCTCCATCCTCCCTGTCTGCGTCTGTAGGGGACAGAGTC
ACC
    Q  I  Q  L  T  Q  S  P  S  S  L  S  A  S  V  G  D  R
V  T

 61
ATCACATGCAGTGCCAGCTCAAGTGTAAATCACATGTTCTGGTATCAGCAGAAGCCC
GGG
    I  T  C  S  A  S  S  S  V  N  H  M  F  W  Y  Q  Q  K
P  G

121
AAAGCCCCCAAACCCTGGATTTATCTCACATCCAACCTGGCTTCTGGAGTCCCTTCA
CGC
    K  A  P  K  P  W  I  Y  L  T  S  N  L  A  S  G  V  P
S  R

181
TTCAGTGGCAGTGGGTCTGGGACAGATTACACTCTCACAATCAGCAGCCTGCAACCT
GAA
    F  S  G  S  G  S  G  T  D  Y  T  L  T  I  S  S  L  Q
P  E

241
GATTTTGCCACTTATTACTGCCAGCAGTGGAGTGGTAACCCGTGGACGTTCGGTCAG
GGC
    D  F  A  T  Y  Y  C  Q  Q  W  S  G  N  P  W  T  F  G
Q  G

301 ACTAAGGTGGAGATCAAA
    T  K  V  E  I  K
```

I. hAQC2 c2 light chain (pAND123) (SEQ ID NOs:53 and 54)

```
  1
CAAATTCAGCTCACCCAGTCTCCATCCTCCCTGTCTGCGTCTGTAGGGGACAGAGTC
ACC
    Q  I  Q  L  T  Q  S  P  S  S  L  S  A  S  V  G  D  R
V  T

 61
ATCACATGCAGTGCCAGCTCAAGTGTAAATCACATGTTCTGGTATCAGCAGAAGCCC
GGG
    I  T  C  S  A  S  S  S  V  N  H  M  F  W  Y  Q  Q  K
P  G

121
AAAGCGCCCAAACTCCTGATTTATCTCACATCCAACCTGGCTTCTGGAGTCCCTTCA
CGC
    K  A  P  K  L  L  I  Y  L  T  S  N  L  A  S  G  V  P
S  R

181
TTCAGTGGCAGTGGGTCTGGGACAGATTACACTCTCACAATCAGCAGCCTGCAACCT
GAA
    F  S  G  S  G  S  G  T  D  Y  T  L  T  I  S  S  L  Q
P  E

241
GATTTTGCCACTTATTACTGCCAGCAGTGGAGTGGTAACCCGTGGACGTTCGGTCAG
GGC
    D  F  A  T  Y  Y  C  Q  Q  W  S  G  N  P  W  T  F  G
Q  G

301 ACTAAGGTGGAGATCAAA
    T  K  V  E  I  K
```

J. chAQC2 unblocked light chain (pAND098) (SEQ ID NOs:55 and 56)

```
  1
GAAATTGTTCTCACCCAGTTTCCAGCACTCATGTCTGCGTCTCCAGGGGAGAAGGTC
5 ACC
    E  I  V  L  T  Q  F  P  A  L  M  S  A  S  P  G  E  K
V T

 61
ATGACCTGCAGTGCCAGCTCAAGTGTAAATCACATGTTCTGGTATCAGCAGAAGCCA
10 AAA
    M  T  C  S  A  S  S  S  V  N  H  M  F  W  Y  Q  Q  K
P K

121
TCCTCCCCCAAACCCTGGATTTATCTCACATCCAACCTGGCTTCTGGAGTCCCTGCT
15 CGC
    S  S  P  K  P  W  I  Y  L  T  S  N  L  A  S  G  V  P
A R

181
TTCAGTGGCAGTGGGTCTGGGACCTCTTACTCTCTCACAATCAGCAGCATGGAGGCT
20 GAA
    F  S  G  S  G  S  G  T  S  Y  S  L  T  I  S  S  M  E
A E

241
GATGCTGCCACTTATTACTGCCAGCAGTGGAGTGGTAACCCGTGGACGTTCGGTGGA
25 GGC
    D  A  A  T  Y  Y  C  Q  Q  W  S  G  N  P  W  T  F  G
G G

301 ACCAAGCTGGAGATCAAA
    T  K  L  E  I  K
```

K. huAQC2 unblocked c1 light chain (pAND150) (SEQ ID NOs:57 and 58)

```
  1
GATATCCAGCTCACCCAGTCTCCATCCTCCCTGTCTGCGTCTGTAGGGGACAGAGTC
5 ACC
    D  I  Q  L  T  Q  S  P  S  S  L  S  A  S  V  G  D  R
V  T

 61
ATCACATGCAGTGCCAGCTCAAGTGTAAATCACATGTTCTGGTATCAGCAGAAGCCC
10 GGG
    I  T  C  S  A  S  S  S  V  N  H  M  F  W  Y  Q  Q  K
P  G

121
AAAGCCCCCAAACCCTGGATTTATCTCACATCCAACCTGGCTTCTGGAGTCCCTTCA
15 CGC
    K  A  P  K  P  W  I  Y  L  T  S  N  L  A  S  G  V  P
S  R

181
TTCAGTGGCAGTGGGTCTGGGACAGATTACACTCTCACAATCAGCAGCCTGCAACCT
20 GAA
    F  S  G  S  G  S  G  T  D  Y  T  L  T  I  S  S  L  Q
P  E

241
GATTTTGCCACTTATTACTGCCAGCAGTGGAGTGGTAACCCGTGGACGTTCGGTCAG
25 GGC
    D  F  A  T  Y  Y  C  Q  Q  W  S  G  N  P  W  T  F  G
Q  G

301 ACTAAGGTGGAGATCAAA
```

T K V E I K

**Example 22**

This example describes the characterization of various AQC2 antibodies of the invention.

*Solid-phase assay for α1 I domain binding.* Fifty µl of 10 mg/ml α1 I domain-GST fusion protein was added to a CORNING COSTAR EASY WASH polystyrene 96-well plate (Gotwals et al., *Biochemistry*, 38, 8280-8 (1999)). Following incubation at 4°C for 16 hrs, the plate was washed four times with 350 µl of 0.1 % Tween-20 in PBS in a plate washer. The plate was blocked by addition of 180 µl of 3% BSA in TBS at 25°C for 60 min, and then washed as above. Dilutions of antibodies (50 µl/well) in TBS containing 1 mg/ml BSA (assay buffer) were prepared in a 96-well roundbottom plate, transferred to the α1 I domain-coated plate, and incubated for 60 min at 25°C. Following a final wash, 100 µl/well of TMB reagent (Pierce) was added. After 10 min, 100 µl of 1 M sulfuric acid was added, and the absorbance at 450 nm was read on a UV-Vis 96-well spectrophotometer.

*Electrochemiluminescence assays for binding of α1β1 integrin or α1 I domain to collagen.* Tosyl-activated DYNABEADS M-280 (Dynal, Inc.) were coated with 100 µg/ml type IV collagen (Sigma) according to the manufacturer's instructions. Cell lysates from α1-transfected K562 cells were prepared as follows. Cells were collected by centrifugation, resuspended at $10^8$ cells/ml in a lysis buffer containing 25 mM Tris, pH 7.4, 1% NP-40, 1 mM $CaCl_2$, 1 mM $MnCl_2$, 1 mM $MgCl_2$, 2% BSA, and 1 mM PMSF, and incubated at 4°C for 60 min. Cell debris was removed by centrifugation at 12,000 rpm for 30 min and the resulting supernatant was used in subsequent experiments. Anti-β1 activating antibody TS2/16 and polyclonal anti-GST antibody (Pharmacia) were labeled with TAG-NHS ester (IGEN International, Inc., Gaithersburg, MD) according to the manufacturer's instructions. Labeled antibodies were purified by gel filtration chromatography on SEPHADEX G25M (Pharmacia).

To carry out the binding assay, collagen-coated beads (1 mg/ml) were blocked for 5 min with 8% Lewis rat plasma in an assay buffer containing 50 mM HEPES, pH 7.5, 150 mM NaCl, and 0.1% Triton X-100. For the α1β1 binding assay,

serial dilutions of antibodies were incubated with 10 μg of beads, cell lysate prepared from $10^5$ α1-transfected K562 cells (*supra*), and 0.1 μg/ml of TAG-TS2/16 in an assay buffer containing 1 mM $MnCl_2$. For the α1 I domain binding assay, the antibodies were incubated with 10 μg of beads, 0.1 μg/ml α1 I domain GST fusion protein, and 1 μg/ml of TAG-anti-GST in an assay buffer containing 1 mM $MnCl_2$. After one to two hours of agitation at room temperature, 200 μl of the assay buffer was added and the samples were read on an ORIGEN 1.5 electrochemiluminescence detector (IGEN). Plots are presented with arbitrary electrochemiluminescence units (ECL) on the ordinate axis.

*Biotinylated mAQC2 competition assay.* A 96-well plate was coated with 50 μl of 5 μg/ml α1 I domain GST fusion protein and blocked with 3% BSA in TBS as described above. Dilutions of antibodies (60 μl/well) in the assay buffer were prepared in a 96-well roundbottom plate, and 60 μl of 0.1 μg/ml biotinylated murine AQC2 in the assay buffer was added. Fifty microliters from each well was transferred to the coated plate and incubated for 3 hrs at 25°C. The plate was then washed as above, 50 μl of 1 μg/ml peroxidase-conjugated EXTRAVIDIN (Sigma) was added, and the plate was incubated another 2 hrs at 25°C. After a final wash, 100 μl/well of TMB reagent (Pierce) was added. After 10 min, 100 μl of 1 M sulfuric acid was added, and the absorbance at 450 nm was read on a UV-Vis 96-well spectrophotometer.

*Experimental results.* The experimental results are shown in Figs. 16A-D and Table 3. The ability of mAQC2, chAQC2, hAQC2, and hAQC2' (i.e., huAQC2-c4; differing from hAQC2 only in that residue 1 of the hAQC2' light chain was D instead of Q) to (1) bind to human α1- transfected K562 cells (by FACS); (2) bind to immobilized α1-I domain (by ELISA); (3) compete with mAQC2 for binding to α1-I domain (ELISA); (4) block α1-I domain binding to collagen (Electrochemiluminescence assay); or (5) block α1β1 integrin binding to collagen (Electrochemiluminescence assay) was determined. The results are shown in Figs. 16A-D, and calculated IC50 (for inhibition) or EC50 (for binding) values are given in Table 3. In each assay, each of the humanized AQC2 forms showed a similar ability to either bind VLA1 (or the α1 domain) or block binding to collagen (Note that in

panel C, the observed difference in intensity between mAQC2 and the humanized forms derives from the use of an anti-murine-IgG secondary antibody, instead of an anti-human-IgG).

**Table 3. Summary of assay results (all values in nM)**

| Antibody | FACS (EC50) | VLA1 Inhibition (IC50) | α1I Inhibition (IC50) | ELISA (EC50) | Competition with biotin-AQC2 (IC50) |
|---|---|---|---|---|---|
| mAQC2 | n.d. | 0.0726 (±0.014) | 0.029 (±0.011) | 0.061 (±0.015) | 38 (±8.7) |
| Chimera | 0.25 | 0.071 (±0.002) | 0.027 (±0.007) | 0.176 (±0.058) | 30 (±6.9) |
| hAQC2 | 0.29 | 0.129 (±0.005) | 0.035 (±0.005) | 0.190 (±0.010) | 65 (±2.2) |
| hAQC2' | 0.43 | 0.125 (±0.018) | 0.037 (±0.001) | 0.313 (±0.072) | 69 (±25.7) |

We next tested whether changes at certain conservative residues in the CDRs could preserve the VLA-1 binding activity of hAQC2. DNA constructs encoding variants of hAQC2 with the following mutations were made by site-directed mutagenesis: (1) G55S in the heavy chain CDR2; (2) S24N in the light chain CDR1 (introducing an occupied N-linked glycosylation site); (3) G92S in the light chain CDR3; (4) a combination of (1) and (2); and (5) a combination of (1) and (3). The DNA constructs encoding both the heavy and light chains were then co-transfected into 293-EBNA cells, and the conditioned medium of the transfectants was assayed for antibody expression by Western blot and ELISA. The results indicated that the hAQC2 variants were expressed as efficiently as cognate hAQC2. FACS analysis using VLA-1-expressing K562 cells further showed that the VLA-1-binding activities

of these variants were similar to hAQC2 itself. In sum, the amino acid substitutions did not alter the VLA-1 binding activity of hAQC2. Indeed, X-ray crystal structure of the RΔH/hAQC2 Fab complex (*infra*) shows that S24 and G92 of the light chain and G55 of the heavy chain are not in the binding pocket that is in contact with the α1-I domain.

**Example 23**

The effector functions of an immunoglobulin couple the immunoglobulin's antigen-binding activity to the inflammatory, cytotoxic and stimulatory arms of the immune system. Effector functions may impair the safety and efficacy of an immunoglobulin therapeutic product. To reduce the potential effector functions of hAQC2, mutations of L234A and L235A were made to its heavy chain to generate hsAQC2. For the same reason, a single mutation of N297Q was made in the heavy chain of hAQC2 to generate an aglycosylated form of hAQC2, named haAQC2. Studies can be done to compare their efficacy, residual effector function, stability and immunogenicity to cognate hAQC2. Unless otherwise indicated, residue position numbers in constant regions as used herein are designated in accordance with the EU numbering convention.

The heavy chain polypeptide sequence of haAQC2 is as follows (Plasmid: pAND161):

```
1    EVQLVESGGG LVQPGGSLRL SCAASGFTFS RYTMSWVRQA
PGKGLEWVAT
51   ISGGGHTYYL DSVKGRFTIS RDNSKNTLYL QMNSLRAEDT
AVYYCTRGFG
101  DGGYFDVWGQ GTLVTVSSAS TKGPSVFPLA PSSKSTSGGT
AALGCLVKDY
151  FPEPVTVSWN SGALTSGVHT FPAVLQSSGL YSLSSVVTVP
SSSLGTQTYI
201  CNVNHKPSNT KVDKKVEPKS CDKTHTCPPC PAPELLGGPS
VFLFPPKPKD
251  TLMISRTPEV TCVVVDVSHE DPEVKFNWYV DGVEVHNAKT
KPREEQYQST
```

301 YRVVSVLTVL HQDWLNGKEY KCKVSNKALP APIEKTISKA
KGQPREPQVY
351 TLPPSRDELT KNQVSLTCLV KGFYPSDIAV EWESNGQPEN
NYKTTPPVLD
401 SDGSFFLYSK LTVDKSRWQQ GNVFSCSVMH EALHNHYTQK SLSLSPG
(SEQ ID NO:5)

The heavy chain polypeptide sequence of hsAQC2 is as follows (Plasmid: pAND171):

1 EVQLVESGGG LVQPGGSLRL SCAASGFTFS RYTMSWVRQA
PGKGLEWVAT
51 ISGGGHTYYL DSVKGRFTIS RDNSKNTLYL QMNSLRAEDT
AVYYCTRGFG
101 DGGYFDVWGQ GTLVTVSSAS TKGPSVFPLA PSSKSTSGGT
AALGCLVKDY
151 FPEPVTVSWN SGALTSGVHT FPAVLQSSGL YSLSSVVTVP
SSSLGTQTYI
201 CNVNHKPSNT KVDKKVEPKS CDKTHTCPPC PAPEAAGGPS
VFLFPPKPKD
251 TLMISRTPEV TCVVVDVSHE DPEVKFNWYV DGVEVHNAKT
KPREEQYNST
301 YRVVSVLTVL HQDWLNGKEY KCKVSNKALP APIEKTISKA
KGQPREPQVY
351 TLPPSRDELT KNQVSLTCLV KGFYPSDIAV EWESNGQPEN
NYKTTPPVLD
401 SDGSFFLYSK LTVDKSRWQQ GNVFSCSVMH EALHNHYTQK SLSLSPG
(SEQ ID NO:6)

**Example 24**

This example describes a method for determining the crystal structure of the complex of a rat/human chimeric α1-I domain of the α1β1 integrin and the hAQC2 Fab fragment.

***Preparation of the protein complex***

The hAQC2 Fab fragment was prepared from hAQC2 antibody using a variation of the procedure of the IMMUNOPURE® Fab preparation kit (Cat# 44885, Pierce, Rockford, IL). The intact hAQC2 antibody was concentrated to 12 mg/ml in a buffer containing 20 mM phosphate, 10 mM EDTA and 25 mM cysteine (pH 7.0). Immobilized papain was added at an enzyme to substrate ratio of 1:50, and digestion was allowed to occur overnight at 37° C. The immobilized papain was removed and the crude digest was dialyzed against 20 mM sodium acetate buffer (pH 4.5). The Fab fragment was separated from residual intact antibody, dimeric Fab fragment, and Fc fragment by cation exchange chromatography using a S-column (Poros HS/M , PERSEPTIVE Biosytems #PO42M26) with a shallow salt gradient. The Fab fragment was then exchanged into 0.1 M Hepes buffer (pH 8.0).

The chimeric α1-I domain used in the present invention is a rat/human chimeric I domain construct (mutant RΔH) containing residues Thr145-Phe336 of the rat α1 integrin chain, where residues Gly217, Arg218, Gln219 and Leu222 (crystal numbering) have been substituted with equivalent human residues Val, Gln, Arg and Arg, respectively, in order to restore antibody binding. The amino acid sequences of chimeric RΔH, rat, and human α1-I domains are given below in SEQ ID NOs:59, 60 and 61, respectively. Recombinant α1-I domain was expressed in *E. coli* as a GST-fusion protein. The RΔH α1-I domain was cleaved with thrombin and purified from a *Pichia pastoris* clone as described previously (Gotwals et al., 1999, *Biochemistry* 38:8280-8288).

```
145  TQLDIV
151  IVLDGSNSIY PWESVIAFLN DLLKRMDIGP KQTQVGIVQY
191  GENVTHEFNL NKYSSTEEVL VAANKIVQRG GRQTMTALGI
231  DTARKEAFTE ARGARRGVKK VMVIVTDGES HDNYRLKQVI
271  QDCEDENIQR FSIAILGHYN RGNLSTEKFV EEIKSIASEP
311  TEKHFFNVSD ELALVTIVKA LGERIF
```

(SEQ ID NO:59)

```
145  TQLDIV
151  IVLDGSNSIY PWESVIAFLN DLLKRMDIGP KQTQVGIVQY
```

191 GENVTHEFNL NKYSSTEEVL VAANKIGRQG GLQTMTALGI
231 DTARKEAFTE ARGARRGVKK VMVIVTDGES HDNYRLKQVI
271 QDCEDENIQR FSIAILGHYN RGNLSTEKFV EEIKSIASEP
311 TEKHFFNVSD ELALVTIVKA LGERIF

(SEQ ID NO:60)

145 TQLDIV
151 IVLDGSNSIY PWDSVTAFLN DLLKRMDIGP KQTQVGIVQY
191 GENVTHEFNL NKYSSTEEVL VAAKKIVQRG GRQTMTALGI
231 DTARKEAFTE ARGARRGVKK VMVIVTDGES HDNHRLKKVI
271 QDCEDENIQR FSIAILGSYN RGNLSTEKFV EEIKSIASEP
311 TEKHFFNVSD EIALVTIVKT LGERIF

(SEQ ID NO:61)

The hAQC2 Fab fragment was mixed with excess chimeric α1-I domain and incubated at 37° C for 15 minutes. The saturated α1/Fab complexes were separated from uncomplexed α1-I domain by size exclusion chromatography using a S200 Sephacryl column (Pharmacia, Gibco). The complex was further concentrated to 11 mg/ml in a 20 mM Tris (pH 7.4), 150 mM NaCl, 1 mM $MnCl_2$, 5 mM β-mercaptoethanol.

***Preparation of crystals***

Crystallization conditions were found using the CRYSTAL SCREEN™ KITs from Hampton Research (Laguna Niguel, CA). Crystals of the complex described above were grown at 20° C by vapor diffusion using an equal amount of protein complex solution and a 20-30% PEG 1500 reservoir solution. Typically, 2 μL of protein complex was added to 2 μL of well solution to yield drops of 4 μL. Crystals grew in two to seven days as hexagonal rods with dimensions 0.8 x 0.05 x 0.05 $mm^3$. The presence of the α1-I domain and hAQC2 Fab fragment was confirmed by SDS-PAGE analysis of dissolved crystals. In order to reduce the inherent radiation damage during data collection, X-ray diffraction data was collected at approximately 100 K. To prepare the crystals for data collection at this low

temperature, crystals were gradually equilibrated into a cryoprotectant solution containing 25% PEG 400 and 30% PEG 1500, and flash cooled in liquid nitrogen.

*Structure determination*

Native X-ray diffraction data to 2.8 Å resolution were collected from a single crystal at about 100 K using an ADSC Quantum 4 charged-coupled device detector at beamline X4A of the Brookhaven National Laboratory (BNL) National Synchrotron Light Source (NSLS). Data was processed using the software programs DENZO and SCALEPACK (Otwinowski & Minor, 1997, *Methods in Enzymol.* 276:307-326). Crystals belonged to the space group $P6_1$ or its enantiomorph $P6_5$, with unit cell dimensions a = b = 255.09 Å, c=38.64 Å. The data set was 96.6% complete and had an R-merge of 8.3%. The Matthews coefficient (Matthews, 1968, J. Mol. Biol. 33:491-497) was 2.59 $Å^3 Da^{-1}$ with a solvent content of 52.1 %, which indicated that there were two complexes in the asymmetric unit. The two complexes in the asymmetric unit were related by non-crystallographic 2-fold symmetry. Data statistics are shown in Table 4.

Molecular replacement searches were done with the program AMoRe (Navaza, 1994, *Acta Cryst.* A50:157-163) from the CCP4 program package (Collaborative Computational Project No.4. The CCP4 Suite: programs for protein crystallography. 1994, *Acta Cryst.* D50:760-763), and molecular graphics manipulations were done with the program QUANTA. A single α1-I domain from the structure of the rat α1-I domain of α1β1 integrin (Protein Data Bank (PDB) accession number 1ck4; Nolte et al., 1999, *FEBS Lett.* 452:379-385) was used as a model or probe for rotation and translation searches. The translation function search indicated that the 1st and 9th highest peaks of the rotation function corresponded to the correct solutions for the two α1-I domains in the asymmetric unit (correlation coefficient (cc) = 21.1%, R=53.1 %) and that the space group was $P6_5$. Subsequently, searches for the hAQC2 Fab fragments were done, keeping the I domain solutions fixed and using a model of the Fv domain of the hAQC2 Fab as a search probe. A clear solution was found for one of the two Fv domains (cc=22.1%, R=52.6 %), but the second Fv could not be located. The position of the second Fv was derived using the non-crystallographic 2-fold symmetry. Rigid body refinement of the two I domains and

two Fv domains reduced the R-factor to 43.6% (R-free = 42.7 %). An 2Fo-Fc electron density map showed clear electron density for the constant domain (Fconst) of the first Fab fragment, but no density for the Fconst domain of the second Fab fragment. A model of the Fconst domain of the first Fab was manually fit in the observed electron density. Subsequent rigid body refinement with the software program CNX (Accelrys Inc., San Diego, CA ©2000; Brunger,1998, *Acta Cryst.* D54:905-921), using data in the 500-2.8 Å resolution range, optimized the position of all domains, reducing the R-factor to 39.7 % (R-free = 38.9%).

All subsequent refinement steps were carried out with the CNX program. To reduce model bias, partial models were used for 2Fo-Fc map calculation and model refinement. The initial partial model, was subjected to simulated annealing and grouped B-factor refinement with non-crystallographic symmetry restraints. The R-working and R-free factors dropped to 28.3% and 32.9%, respectively. Several cycles consisting of iterative model building, maximum likelihood positional refinement and B-factor refinement followed. Only model adjustments that resulted in a drop in the R-free factor were accepted. A bulk-solvent correction was employed after the complete model was built. The R-working and R-free factors of the final model are 21.3 % and 27.2 %, respectively for the data ($F > 2\sigma$) in the 500-2.8 Å resolution range.

The final 2Fo-Fc electron density map is of good quality for most of the complex with the exception of amino acid residues 288-295 of one I domain fragment (molecule A in Fig. 19) that are associated with weak electron density and have not been included in the model. In addition, the entire constant domain of one Fab fragment has no visible electron density, which indicates that it is disordered. This appears to be consequence of the absence of crystal contacts for the constant domain of the Fab fragment due to its position within a large solvent channel. This domain was also not included in the final model that consists of 1030 amino acid residues, constituting 6 polypeptide chains, and 2 manganese ions. The r.m.s. positional deviation between equivalent residues from the two complexes in the asymmetric unit is small (0.37 Å for 1660 equivalent main chain atoms). Stereochemistry statistics were calculated with the software programs PROCHECK

(Laskowski et al., 1993, *J. Appl. Cryst.* 26:283-291; Morris et al., 1992, *Proteins* 12:345-364) and CNX. Hydrogen bonds (< 3.6 Å) were found with the program CONTACT (Tadeusz Skarzynski, Imperial College, London, 1.12.88; Collaborative Computational Project No.4 . The CCP4 Suite: programs for protein crystallography. 1994, *Acta Cryst.* D50, 760-763). All non-glycine residues (except residue Thr50 of the L chain that will be discussed below) are in the allowed regions of the Ramachandran diagram and 86% of the residues are in the most favored regions. The average B-factor of the main chain atoms is 38.5 $Å^2$. Crystallographic analysis data are in Table 4.

**Table 4: Summary of Data Statistics and Crystallographic Analysis**

| | | |
|---|---|---|
| **Data collection** | | |
| Cell dimensions a, b, c ( Å ) | | 255.09 , 255.09, 38.64 |
| Space group | | $P6_5$ |
| Resolution ( Å ) | | 500-2.8 (2.9-2.8)† |
| Unique reflections | | 35275 |
| Completeness (%) | | 96.6 (87.7)† |
| Average I/s | | 11.92 (2.29)† |
| Rmerge*(%) | | 8.3 (30.9)† |
| **Model** | | |
| Number of non-H atoms | | 7950 |
| Number of protein residues | | 1030 |
| Contents of asymmetric unit | | 2 I domains, 1 Fab fragment, 1 Fv domain |
| Average B-factor ($Å^2$) | | 38.5 |
| **Refinement** | | |
| Resolution range used | (F>2σ) | 500-2.8 |
| R-factor (R-working) (%) | | 21.3 |
| R-free††(%) | | 27.2 |
| **Stereochemistry** | | |
| RMS deviations | | |
| Bond lengths (Å) | | 0.007 |
| Angles (°) | | 1.43 |

* Rmerge = $\Sigma_h \Sigma_i |I_{hi} - I_h| / \Sigma_{hi} I_{hi}$

† Values for the highest resolution shell given in parenthesis.

†† 8% of the data were allocated for the calculation of R-free factor.

**Example 25**

This example describes the crystal structure of the complex of a rat/human chimeric α1-I domain of the α1β1 integrin and the hAQC2 Fab fragment.

*Architecture of Crystal Structure*

The crystal structure of the complex of the rat/human chimeric α1-I domain of the α1β1 integrin and the hAQC2 Fab fragment has an elongated shape (Fig. 20). The dimensions of the complex are 100 Å x 50 Å x 35 Å.

The Fab fragment exhibits the typical immunoglobulin fold. The light chain and heavy chains of the Fab fragment each form two broad sheets of anti-parallel β-strands which pack tightly together to form a scaffold for the complementarity determining region (CDR) loops which extend from the packed sheets. Both the light chain and the heavy chain contain three CDR loops. The light chain loops are called L1, L2 and L3, while the heavy chain loops are referred to as H1, H2 and H3. The complementarity determining region (CDR) loops correspond to canonical structure 1 for light chain L1, L2 and L3 loops and for heavy chain H1 and H2 loops (Chothia et al., 1989, Nature 342:877-883). The heavy chain H3 loop has a tight β-hairpin-like conformation that is stabilized by internal hydrogen bonds as well as two aromatic residues (Tyr104 and Phe105) that are packed against the light chain. Residue Thr50 of L2 adopts mainchain dihedral angles that fall in the disallowed regions of the Ramachandran diagram. The same observation for the corresponding residue has been made for other antibodies (Muller et al., 1998, *Structure* 6, pp.1153-11567) which indicates that this is a natural characteristic of L2 loops.

The α1-I domain in the present invention has a structure very similar to the uncomplexed α1-I domain (PDB accession number 1ck4; Nolte et al., 1999, FEBS Lett. 452:379-385; PDB accession code 1qc5; Rich et al.,1999, *J. Biol. Chem.* 274:24906-24913). The I domain structure exhibits a "dinucleotide-binding" or "Rossman" fold (Rao & Rossman, 1973, J. Mol. Biol. 76:241-256) in which a central sheet of five parallel β-strands and one small antiparallel-strand is surrounded on both sides by a total of seven α-helices. The six β-strands of the structure in this invention will be referred to as βA, βB, βC, βD, βE, and βF and the seven α-helices are called α1, α2, α3, α4, α5, α6 and α7.

Three characteristic structural features exist for I domains. The first characteristic feature is the presence of an inserted small helix in the βE-α6 loop, termed as the C helix. Most of the C helix loop of molecule A (Fig. 19) in the present invention is associated with weak electron density, which suggests disorder. This appears to be a consequence of absence of crystal contacts or contacts with the Fab that would have stabilized the loop. However, the same loop in molecule B (Fig. 19) in the present invention has well-defined electron density and has been included in the model. The second characteristic feature of α1-I domains is the MIDAS or Metal-Ion-Dependent-Adhesion-Site where metal ions and ligands are implicated to bind to the I domain. Five key residues which form part of the MIDAS are referred to as the "DxSxS-T-D" motif. These residues, which are completely conserved among I domains, coordinate the metal ion (Gotwals et al., 1999, *Biochemistry* 38:8280-8288). The crystals in the present invention were grown in the presence of manganese and the MIDAS site of the I domain in this structure is observed to contain a $Mn^{+2}$ metal ion. The ion is directly coordinated by the side chains of residues Ser156, Ser158 and Thr224. The 2Fo-Fc electron density map shows no evidence that MIDAS residues Asp154 and Asp257 make water-mediated indirect coordination of the metal ion (Fig. 20). However, the apparent absence of water molecules could be a consequence of the limited resolution (2.8 Å) of the electron density map. The third feature of I domains is that all determined structures of I domains belong to one of two conformations called "open" and "closed". The differences between the open and closed conformation include a different mode of metal ion coordination and a significant (about 10 Å) positional shift of the C-terminal helix of the I domain. The I domain in the complex in the present invention is in the closed conformation.

In the structure of the complex in the present invention, the Fab fragment binds to its epitope on the front upper surface of the I domain with a footprint 35 Å by 30 Å. The total buried surface area in the antibody-antigen interface is 1534 $Å^2$ which is typical of other antibody-antigen complexes (Davies et al., 1996, *Proc. Natl. Acad. Sci. USA* 93:7-12; Jones & Thornton, 1996, *Proc. Natl. Acad. Sci. USA* 93:13-20). The surface is 25% hydrophobic and 75% hydrophilic in character. The heavy chain contributes 65% of the buried surface area for the complex, while the

remaining 35% is contributed by the light chain. The antibody epitope consists of residues located in four loops of the I domain (Emsley et al., 2000, *Cell* 101:47-56). Three of the loops form the MIDAS site: loop 1 (βA- α1) which contains the conserved DXSXS sequence, loop 2 (α3-α4) which contains the MIDAS Thr224 and loop 3 (βD-α5) that contains MIDAS residue Asp257. The fourth loop is the C-helix loop and is involved in only in minor contacts.

The central feature of the antigen-antibody interaction is the coordination of the MIDAS site metal ion by Asp101 from the CDR H3 of the antibody (Fig. 20). The distance between the ion and Oδ1 of Asp101 is 2.4 Å. In addition, the Oδ2 atom of Asp101 is interacting with His261 of the I domain. Interestingly, the CDR H3 contains several glycine residues adjacent to Asp101 (sequence GFGDGGY)(SEQ ID NO:62), presumably to allow enough flexibility to the CDR loop to permit proper coordination of the metal ion. The CDR H3 sequence is essentially invariant in monoclonal antibodies that were raised against the same antigen and found to belong in the same class. Most of the antibody residues that are involved in antibody-antigen contacts are located in L3, H1, H2 and H3 CDR loops. A few residues from the L1 (Asn30) and L2 (Tyr48) loops appear to form minor Van Der Waals contacts. L3 primarily contributes to contacts through two large hydrophobic residues, Trp90 and Trp95. In addition, Asn93 from L3 forms hydrogen bonds with Gln223 of the I domain. The side chains of His56 and Tyr58 from the H2 loop form hydrogen bonds with main chain atoms of loop 2 of the I domain. Arg31 of H1 is in contact with Arg291 of loop 4 of the I domain. Arg222 from loop 2 of the I domain is sandwiched between several antibody residues including Tyr58, Trp95 and Asn93. This is the only residue out of the four mutated in the RΔH I domain, that is involved in contacts with the Fab. It is therefore likely to be the only residue responsible for restoring the binding of the antibody after the mutagenesis.

***Comparison of the crystal structure of the complex of a rat/human chimeric α1-I domain and the hAQC2 Fab fragment with other I domain structures***

The chimeric RΔH α1-I domain has four sequence differences with the rat α1-I domain (rat residues: 217G, 218R, 219Q and 222L), eight sequence differences with the human α1-I domain (human residues: 163D, 166T, 214K, 264H,

268K, 288S, 322I and 380T), and ten sequence differences with the clone used in the crystal structure studies of human α1-I domain (clone residues: 163D, 166T, 174E, 214K, 230I, 264H, 268K, 288S, 322I and 380T). In the unliganded rat α1β1 α1-I domain crystal structure (PDB accession code 1ck4; Nolte et al., 1999, *FEBS Lett.* 452:379-385), the α1-I domain contains no bound metal ions and adopts the "closed" conformation. In the unliganded human α1-I domain crystal structure (accession code 1qc5; Rich et al., 1999, *J. Biol. Chem.* 274:24906-24913), the α1-I domain contains bound $Mg^{+2}$ and similarly adopts the closed conformation. Superimposition of these two structures with the complexed chimeric α1-I domain indicates that there are only minor conformational changes upon hAQC2 antibody binding. The r.m.s. positional deviation between the rat and chimeric α1-I domain is 1.04 Å for all 768 main chain atoms. The r.m.s. positional deviation between the human and chimeric α1-I domain is 0.69 Å for all 764 main chain atoms. The biggest differences (human and chimeric α1-I domain pair) are observed in loop 1 (r.m.s. deviations 1.24 Å for main chain atoms of residues 154-161) and the loop 4 (C helix loop) of the α1-I domain (r.m.s. deviations 1.55 Å for main chain atoms of residues 288-296). However, these differences can be more accurately described as shifts of the whole secondary structure elements rather than complex conformational changes. These are likely to be within the normal range of conformational flexibility of proteins. The r.m.s. positional deviation between the human and chimeric α1-I domain for backbone atoms of amino acid residues Glu192, Gln218, Arg219, Gly220, and Gly221 (crystal numbering) is 0.33 Å. The r.m.s. positional deviation between the rat and chimeric α1-I domain for backbone atoms of amino acid residues Asp154, Ser156, Asn157, Ser158, Tyr160, Glu192, Gln218, Arg219, Gly220, Gly221, Arg222, Gln223, Thr224, Asp257, His261, Asn263, Arg291, and Leu294 (crystal numbering) is 0.97 Å.

The I domain maintains the "closed" I domain conformation that has been observed only for unliganded I domains crystallized in the absence of ligands or pseudo-ligands bound to the MIDAS site. The r.m.s. positional deviation of the C-terminal helices of the human and chimeric I domains (calculated for the main chain atoms of residues 321-335) is 0.64 Å. A simulated annealing omit map calculated for the final refined model unambiguously confirms that the position of the

C-terminal helix and adjacent structural elements are consistent with the closed conformation.

In order to investigate the effects of ligand binding to the modes of metal ion coordination, the structure of the present invention was superimposed with the structures of the unliganded α2-I domain (PDB accession code 1aox; Emsley et al., 1997, *J. Biol. Chem.* 272:28512-28517) and the α2-I domain complexed with a collagen peptide (PDB accession code 1dzi; Emsley et al., 2000, *Cell* 101:47-56). The coordination of the metal ion by Asp101 from the antibody is remarkably similar to the coordination of the metal ion of the α2-I domain by a glutamic acid from the collagen peptide. Another feature that is conserved is the simultaneous interaction of the acidic group with His261 (His258 in the α2-I domain). All MIDAS residues of the I domain-Fab complex except Ser156 and Ser158 adopt conformations very similar to those observed in the unliganded I domain. In contrast, the side chains of Ser156 and Ser158, as well as the metal, adopt conformations similar with those of the liganded I domain. It is clear that the coordination of the metal ion by Asp101 does not allow the ion to maintain the position and coordination distances that are observed in the unliganded state. Thus, the metal ion is not directly coordinated by Asp257, a fact that permits the ion to maintain high electrophilicity.

***Biological Implications***

In the present invention, there is no direct coordination of the metal by Asp257, which may permit high affinity binding by lowering the energy barrier between a closed (no ligand bound) and open (ligand bound) conformation. However, the coordination of the metal by an aspartic acid from the antibody is not sufficient to induce the open conformation to the I domain in the present invention. The I domain - Fab complex structure indicates that it is possible to have strong binding to the I domain that adopts the closed conformation and that coordination of the metal ion by an acidic residue from the ligand may be necessary but not sufficient to induce a conformational change to the open state. Binding of the antibody is expected to stabilize the low affinity state of the integrin and prevent the outside-in signaling that would have accompanied integrin binding to collagen.

Although the foregoing invention has been described in some detail by way of illustration and example for purposes of clarity of understanding, it will be apparent to those skilled in the art that certain changes and modifications will be practiced. Therefore, the description and examples should not be construed as limiting the scope of the invention.

What is claimed is:

1. An anti-VLA-1 antibody whose light chain complementarity determining regions are defined by amino acid residues 24 to 33, 49 to 55, and 88 to 96 of SEQ ID NO:1, and whose heavy chain complementarity determining regions are defined by amino acid residues 31 to 35, 50 to 65, and 98 to 107 of SEQ ID NO:2.

2. The antibody of claim 1, wherein the antibody comprises a light chain variable domain sequence of SEQ ID NO:1 and a heavy chain variable domain sequence of SEQ ID NO:2.

3. The antibody of claim 1, wherein the antibody comprises the same heavy and light chain polypeptide sequences as an antibody produced by hybridoma mAQC2 (ATCC accession number PTA3273).

4. The antibody of claim 1, wherein the antibody is a humanized antibody.

5. The antibody of claim 4, wherein the antibody comprises at least one of the following residues in its light chain: Q1, L4, P46, W47 and Y71; or at least one of the following residues in its heavy chain: D1, V12, S28, F29, A49, T93, R94 (Kabat numbering convention).

6. The antibody of claim 4, wherein the antibody comprises a light chain variable domain sequence defined by amino acid residues 1 to 106 of SEQ ID NO:3, and a heavy chain variable domain sequence defined by amino acid residues 1 to 118 of SEQ ID NO:4.

7. The antibody of claim 4, wherein the antibody comprises the same heavy and light chain polypeptide sequences as an antibody produced by cell line hAQC2 (ATCC accession number PTA3275).

8. The antibody of claim 4, wherein the heavy chain is mutated at one or more of amino acid residues selected from the group consisting of residues 234, 235, 236, 237, 297, 318, 320 and 322 (EU numbering system), thereby causing an alteration in an effector function while retaining binding to VLA-1 as compared with an unmodified antibody.

9. The antibody of claim 8, wherein the antibody comprises the mutations L234A and L235A (EU numbering system) in its heavy chain as compared with an unmodified antibody.

10. The antibody of claim 4, wherein the antibody comprises the same heavy and light polypeptide sequences as an antibody produced by cell line hsAQC2 (ATCC accession number PTA3356).

11. The antibody of claim 4, wherein the antibody is mutated at an amino acid residue that is a glycosylation site, thereby eliminating the glycosylation site.

12. The antibody of claim 11, wherein the antibody comprises the mutation N297Q in its heavy chain (EU numbering system).

13. The antibody of claim 4, wherein the antibody comprises the same heavy and light chain polypeptide sequences as an antibody produced by cell line haAQC2 (ATCC accession number PTA3274).

14. A composition comprising an antibody of any one of claims 4-13, and a pharmaceutically acceptable carrier.

15. An isolated nucleic acid comprising a coding sequence for SEQ ID NO:1.

16. An isolated nucleic acid comprising a coding sequence for SEQ ID NO:2.

17. An isolated nucleic acid comprising a coding sequence for the light chain of an antibody produced by hybridoma mAQC2 (ATCC accession number PTA3273).

18. An isolated nucleic acid comprising a coding sequence for the heavy chain of an antibody produced by hybridoma mAQC2 (ATCC accession number PTA3273).

19. An isolated nucleic acid comprising a coding sequence for the light chain of an antibody produced by cell line hAQC2 (ATCC accession number PTA3275).

20. An isolated nucleic acid comprising a coding sequence for the heavy chain of an antibody produced by cell line hAQC2 (ATCC accession number PTA3275).

21. An isolated nucleic acid comprising a coding sequence for the heavy chain of an antibody produced by cell line haAQC2 (ATCC accession number PTA3274).

22. An isolated nucleic acid comprising a coding sequence for the heavy chain of an antibody produced by cell line hsAQC2 (ATCC accession number PTA3356).

23. An isolated nucleic acid comprising a coding sequence for residues 1 to 106 of SEQ ID NO:3.

24. An isolated nucleic acid comprising a coding sequence for residues 1 to 118 of SEQ ID NO:4.

25. A method of treating a subject with an immunological disorder mediated by VLA-1, comprising administering to the subject the composition of claim 14.

26. A method of determining the level of VLA-1 in a tissue, comprising contacting the tissue with the antibody of claim 1, and detecting the binding of the antibody to the tissue, thereby determining the level of VLA-1 in the tissue.

27. A cell of hybridoma mAQC2 (ATCC accession number PTA3273).

28. A cell of cell line hAQC2 (ATCC accession number PTA3275).

29. A cell of cell line haAQC2 (ATCC accession number PTA3274).

30. A cell of cell line hsAQC2 (ATCC accession number PTA3356).

31. A computer for producing a three-dimensional representation of:

(a) a molecular complex, wherein said molecular complex is defined by the set of structure coordinates of a complex of a chimeric I domain of a $\alpha 1\beta 1$ integrin RΔH and a humanized antibody hAQC2, according to Fig. 19; or

(b) a homologue of said molecular complex, said homologue having a root mean square deviation from the backbone atoms of said amino acids of not more than 0.65 Å;

wherein said computer comprises:

(i) a machine-readable data storage medium comprising a data storage material encoded with machine-readable data, wherein said data comprises at least a portion of the structure coordinates of said complex, according to Fig. 19;

(ii) a working memory for storing instructions for processing said machine-readable data;

(iii) a central-processing unit coupled to said working memory and to said machine-readable data storage medium for processing said machine-readable data storage medium for processing said machine readable data into said three-dimensional representations; and

(iv) a display coupled to said central-processing unit for displaying said three-dimensional representation.

32. A computer for producing a three-dimensional representation of a molecule or molecular complex comprising:

a) a first binding site defined by structure coordinates of hAQC2 amino acids comprising at least seven of light chain residues Asn30, Tyr48, Trp90, Ser91, Asn93 and Trp95, and heavy chain residues Ser30, Arg31, Trp47, Ser52, Gly53, His56, Tyr58, Phe99, Gly100 and Asp101 according to Fig. 19; or

b) a homologue of said molecule or molecular complex, wherein said homologue comprises a second binding site that has a root mean square deviation from the backbone atoms of the hAQC2 amino acids of not more than 1.10 Å; and wherein said computer comprises:

(i) a machine-readable data storage medium comprising a data storage material encoded with machine-readable data, wherein said data comprises the structure coordinates of hAQC2 amino acids comprising at least seven light chain residues Asn30, Tyr48, Trp90, Ser91, Asn93 and Trp95, and heavy chain residues Ser30, Arg31, Trp47, Ser52, Gly53, His56, Tyr58, Phe99, Gly100 and Asp101 according to Fig. 19; and

(ii) a working memory for storing instructions for processing said machine-readable data;

(iii) a central-processing unit coupled to said working memory and to said machine-readable data storage medium for processing said machine-readable data storage medium for processing said machine readable data into said three-dimensional representations;

(iv) a display coupled to said central-processing unit for displaying said three-dimensional representation.

33. A computer for producing a three-dimensional representation of:

(a) a first binding site defined by structure coordinates of hAQC2 amino acids comprising at least seven of light chain residues Asn30, Tyr48, Trp90, Ser91, Asn93 and Trp95, and heavy chain residues Ser30, Arg31, Trp47, Ser52, Gly53, His56, Tyr58, Phe99, Gly100 and Asp101, according to Fig. 19; or

(b) a second binding site of a homologue that has a root mean square deviation from the backbone atoms of the hAQC2 amino acids of not more than 1.10 Å;

wherein said computer comprises:

(i) a machine-readable data storage medium comprising a data storage material encoded with machine-readable data, wherein said data comprises the structure coordinates of hAQC2 amino acid acids selected from a group comprising at least seven of light chain residues Asn30, Tyr48, Trp90, Ser91, Asn93 and Trp95, and heavy chain residues Ser30, Arg31, Trp47, Ser52, Gly53, His56, Tyr58, Phe99, Gly100 and Asp101, according to Fig. 19;

(ii) a working memory for storing instructions for processing said machine-readable data;

(iii) a central-processing unit coupled to said working memory and to said machine-readable data storage medium for processing said machine-readable data storage medium for processing said machine readable data into said three-dimensional representations;

(iv) a display coupled to said central-processing unit for displaying said three-dimensional representation.

34. A method for identifying an inhibitor of an I domain of an integrin comprising the steps of:

(a) using structure coordinates of hAQC2 amino acids comprising at least seven of light chain residues Asn30, Tyr48, Trp90, Ser91, Asn93 and Trp95, and heavy chain residues Ser30, Arg31, Trp47, Ser52, Gly53, His56, Tyr58, Phe99, Gly100 and Asp101, according to Fig. 19 or ± a root mean square deviation from the backbone atoms of said hAQC2 amino acids not more than 1.10 Å, to generate a three-dimensional structure of a binding site;

(b) employing said three-dimensional structure to design or select a potential antagonist;

(c) synthesizing said potential antagonist; and

(d) contacting said potential antagonist with hAQC2 to determine the ability of said potential antagonist to interact with hAQC2, wherein the ability of said potential antagonist to interact with hAQC2 indicates that the potential antagonist is an inhibitor of the I domain.

35. An inhibitor of I domain of integrin identified by the method according to claim 34.

36. A computer for producing a three-dimensional representation of a molecule or molecular complex comprising:

a) a first binding site defined by structure coordinates of I domain amino acid residues Asp154, Ser156, Asn157, Ser158, Tyr160, Glu192, Gln218, Arg219, Gly220, Gly221, Arg222, Gln223, Thr224, Asp257, His261, Asn263, Arg291, and Leu294, according to Fig. 19; or

b) a homologue of said molecule or molecular complex, wherein said homologue comprises a second binding site that has a root mean square deviation from the backbone atoms of said I domain amino acids not more than 0.92 Å;

wherein said computer comprises:

(i) a machine-readable data storage medium comprising a data storage material encoded with machine-readable data, wherein said data comprises the

structure coordinates of I domain amino acid residues Asp154, Ser156, Asn157, Ser158, Tyr160, Glu192, Gln218, Arg219, Gly220, Gly221, Arg222, Gln223, Thr224, Asp257, His261, Asn263, Arg291, and Leu294, according to Fig. 19; and

(ii) a working memory for storing instructions for processing said machine-readable data;

(iii) a central-processing unit coupled to said working memory and to said machine-readable data storage medium for processing said machine-readable data storage medium for processing said machine readable data into said three-dimensional representations; and

(iv) a display coupled to said central-processing unit for displaying said three-dimensional representation.

37. A computer for producing a three-dimensional representation of:

(a) a first binding site defined by structure coordinates of I domain amino acids residues Asp154, Ser156, Asn157, Ser158, Tyr160, Glu192, Gln218, Arg219, Gly220, Gly221, Arg222, Gln223, Thr224, Asp257, His261, Asn263, Arg291, and Leu294, according to Fig. 19; or

(b) a second binding site of a homologue that has a root mean square deviation from the backbone atoms of said I domain amino acids not more than 0.92 Å;

wherein said computer comprises:

(i) a machine-readable data storage medium comprising a data storage material encoded with machine-readable data, wherein said data comprises structure coordinates of I domain amino residues Asp154, Ser156, Asn157, Ser158, Tyr160, Glu192, Gln218, Arg219, Gly220, Gly221, Arg222, Gln223, Thr224, Asp257, His261, Asn263, Arg291, and Leu294, according to Fig. 19; and

(ii) a working memory for storing instructions for processing said machine-readable data;

(iii) a central-processing unit coupled to said working memory and to said machine-readable data storage medium for processing said

machine-readable data storage medium for processing said machine readable data into said three-dimensional representations; and

(iv) a display coupled to said central-processing unit for displaying said three-dimensional representation;

38. A computer for producing a three-dimensional representation of a molecule or molecular complex comprising:

a) a first binding site defined by structure coordinates of I domain amino acids comprising at least three of residues Glu192, Gln218, Arg219, Gly220, and Gly221, according to Fig. 19; or

b) a homologue of said molecule or molecular complex, wherein said homologue comprises a second binding site that has a root mean square deviation from the backbone atoms of said I domain amino acids not more than 0.30 Å;

wherein said computer comprises:

(i) a machine-readable data storage medium comprising a data storage material encoded with machine-readable data, wherein said data comprises the structure coordinates of I domain amino acids comprising at least three of residues Glu192, Gln218, Arg219, Gly220, and Gly221, according to Fig. 19; and

(ii) a working memory for storing instructions for processing said machine-readable data;

(iii) a central-processing unit coupled to said working memory and to said machine-readable data storage medium for processing said machine-readable data storage medium for processing said machine readable data into said three-dimensional representations; and

(iv) a display coupled to said central-processing unit for displaying said three-dimensional representation;

39. A computer for producing a three-dimensional representation of:

(a) a first binding site defined by structure coordinates of I domain amino acids comprising at least three of residues Glu192, Gln218, Arg219, Gly220, and Gly221, according to Fig. 19; or

(b) a second binding site of a homologue that has a root mean square deviation from the backbone atoms of said I domain amino acids not more than 0.30 Å;

wherein said computer comprises:

(i) a machine-readable data storage medium comprising a data storage material encoded with machine-readable data, wherein said data comprises the structure coordinates of I domain amino acids comprising at least three of residues Glu192, Gln218, Arg219, Gly220, and Gly221, according to Fig. 19;

(ii) a working memory for storing instructions for processing said machine-readable data;

(iii) a central-processing unit coupled to said working memory and to said machine-readable data storage medium for processing said machine-readable data storage medium for processing said machine readable data into said three-dimensional representations; and

(iv) a display coupled to said central-processing unit for displaying said three-dimensional representation;

40. A method for identifying an inhibitor of an I domain of an integrin comprising the steps of:

(a) using the structure coordinates of I domain amino acids residues Asp154, Ser156, Asn157, Ser158, Tyr160, Glu192, Gln218, Arg219, Gly220, Gly221, Arg222, Gln223, Thr224, Asp257, His261, Asn263, Arg291, and Leu294, according to Fig. 19, to generate a three-dimensional structure of a binding site;

(b) employing said three-dimensional structure to design or select a potential antagonist;

(c) synthesizing said potential antagonist; and

(d) contacting said potential antagonist with I domain to determine the ability of said potential antagonist to interact with I domain, wherein the ability of

said potential antagonist to interact with the I domain indicates that the potential antagonist is an inhibitor of the I domain.

41. A method for identifying an inhibitor of an I domain of an integrin comprising the steps of:

(a) using the structure coordinates of at least three of I domain amino acids comprising residues Glu192, Gln218, Arg219, Gly220, and Gly221, according to Fig. 19, or ± a root mean square deviation from the backbone atoms of said I domain amino acids not more than 0.30 Å, to generate a three-dimensional structure of a binding site;

(b) employing said three-dimensional structure to design or select a potential antagonist;

(c) synthesizing said potential antagonist; and

(d) contacting said potential antagonist with I domain to determine the ability of said potential antagonist to interact with I domain of integrin, wherein the ability of said potential antagonist to interact with the I domain indicates that the potential antagonist is an inhibitor of the I domain.

42. An inhibitor of I domain of integrin identified by the method according to any one of claims 40 and 41.

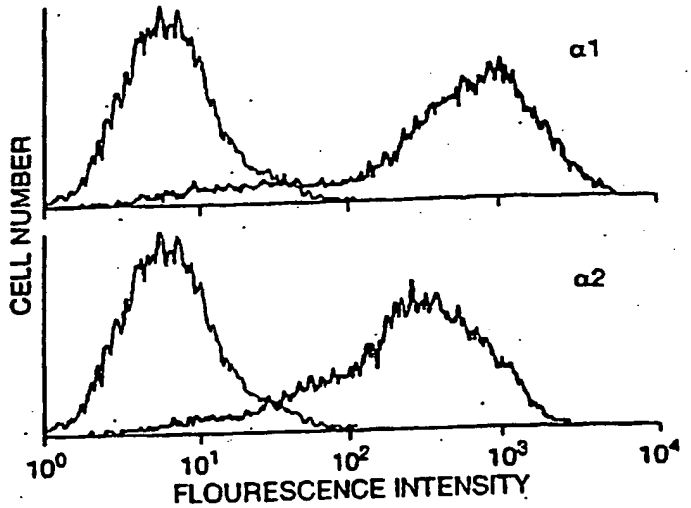

α1
α2
CELL NUMBER
$10^0$
$10^1$
$10^2$
$10^3$
$10^4$
FLOURESCENCE INTENSITY

FIG. 1A

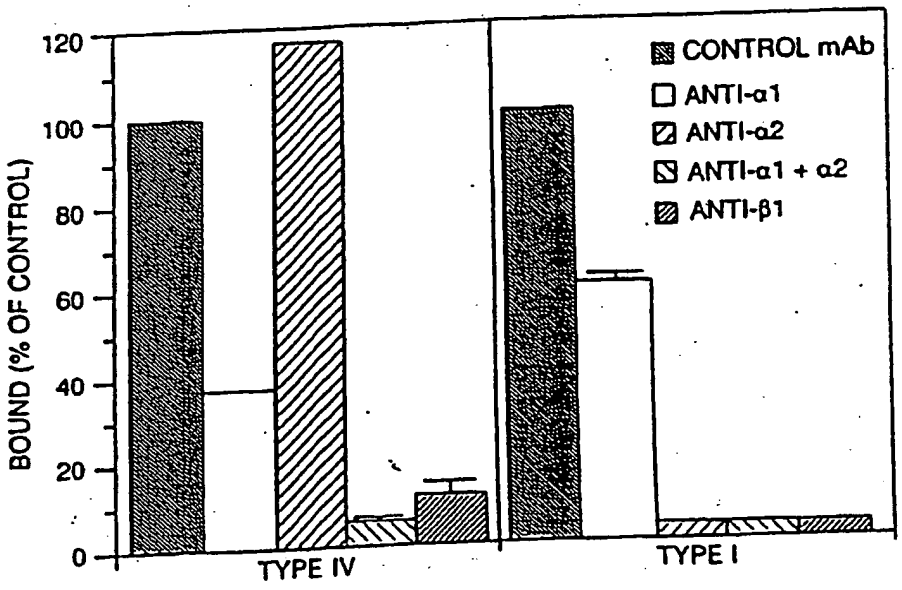

120
100
80
60
40
20
0
BOUND (% OF CONTROL)
TYPE IV
TYPE I
CONTROL mAb
ANTI-α1
ANTI-α2
ANTI-α1 + α2
ANTI-β1

FIG. 1B

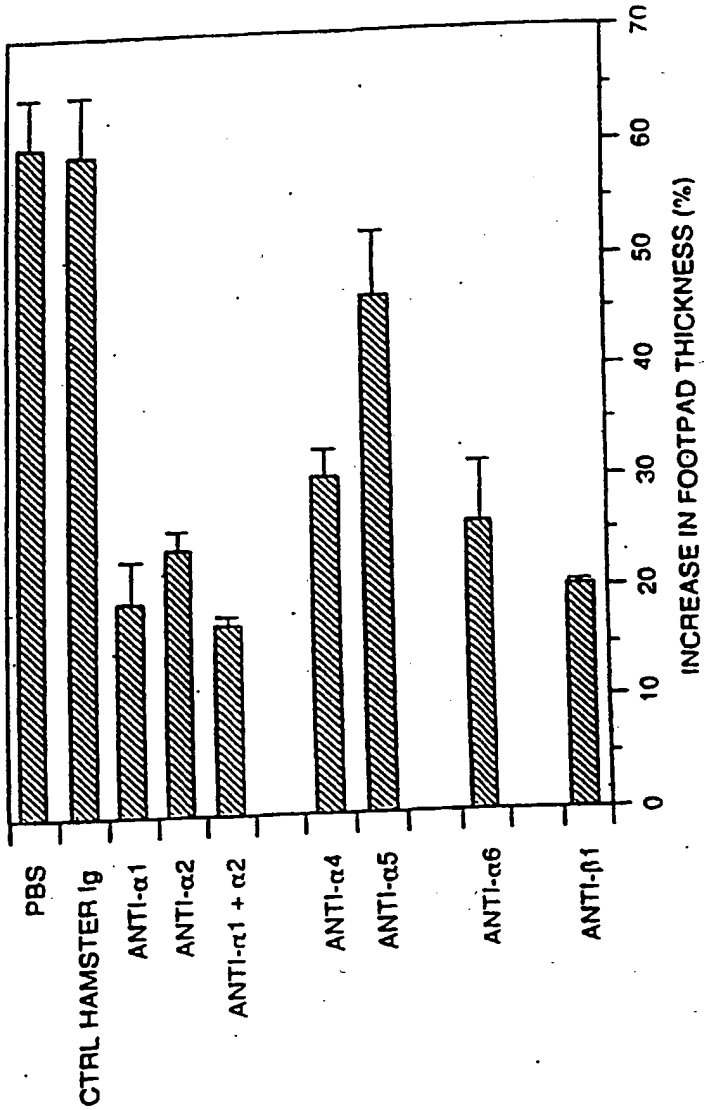

INCREASE IN FOOTPAD THICKNESS (%)
0
10
20
30
40
50
60
70
PBS
CTRL HAMSTER Ig
ANTI-α1
ANTI-α2
ANTI-α1 + α2
ANTI-α4
ANTI-α5
ANTI-α6
ANTI-β1

FIG. 2

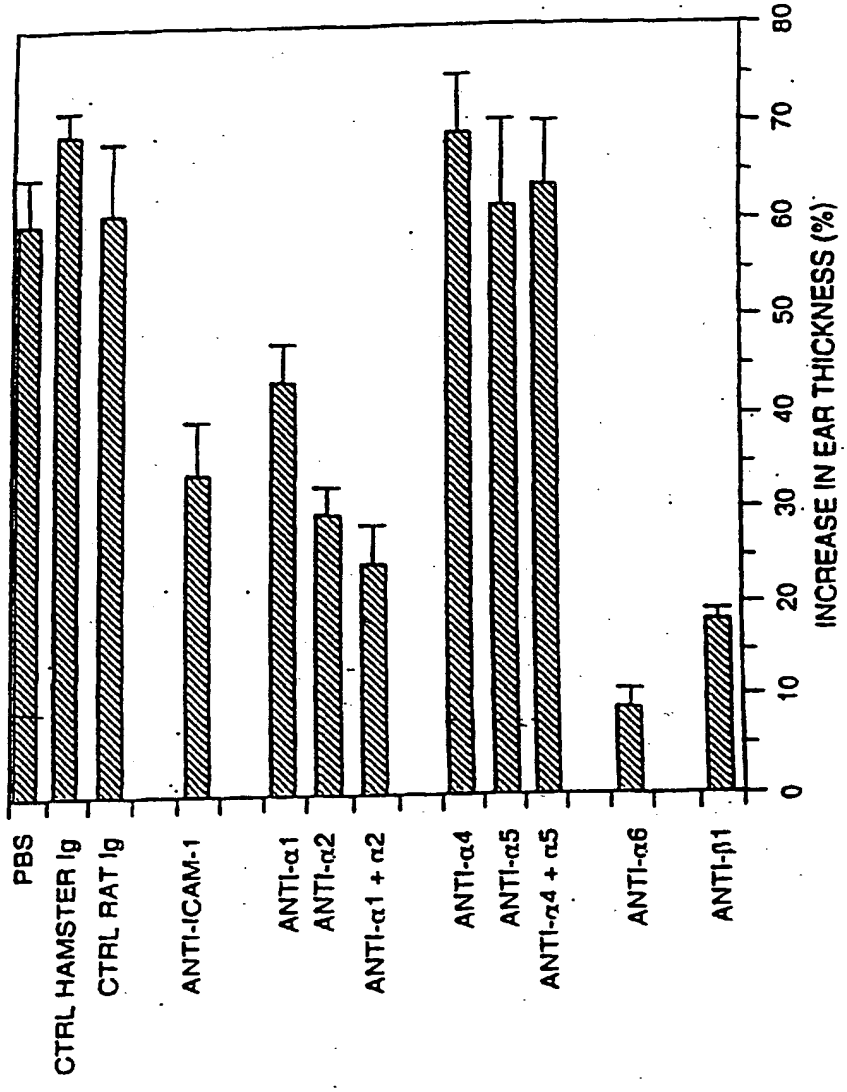

INCREASE IN EAR THICKNESS (%)
0
10
20
30
40
50
60
70
80
PBS
CTRL HAMSTER Ig
CTRL RAT Ig
ANTI-ICAM-1
ANTI-α1
ANTI-α2
ANTI-α1 + α2
ANTI-α4
ANTI-α5
ANTI-α4 + α5
ANTI-α6
ANTI-β1

FIG. 3

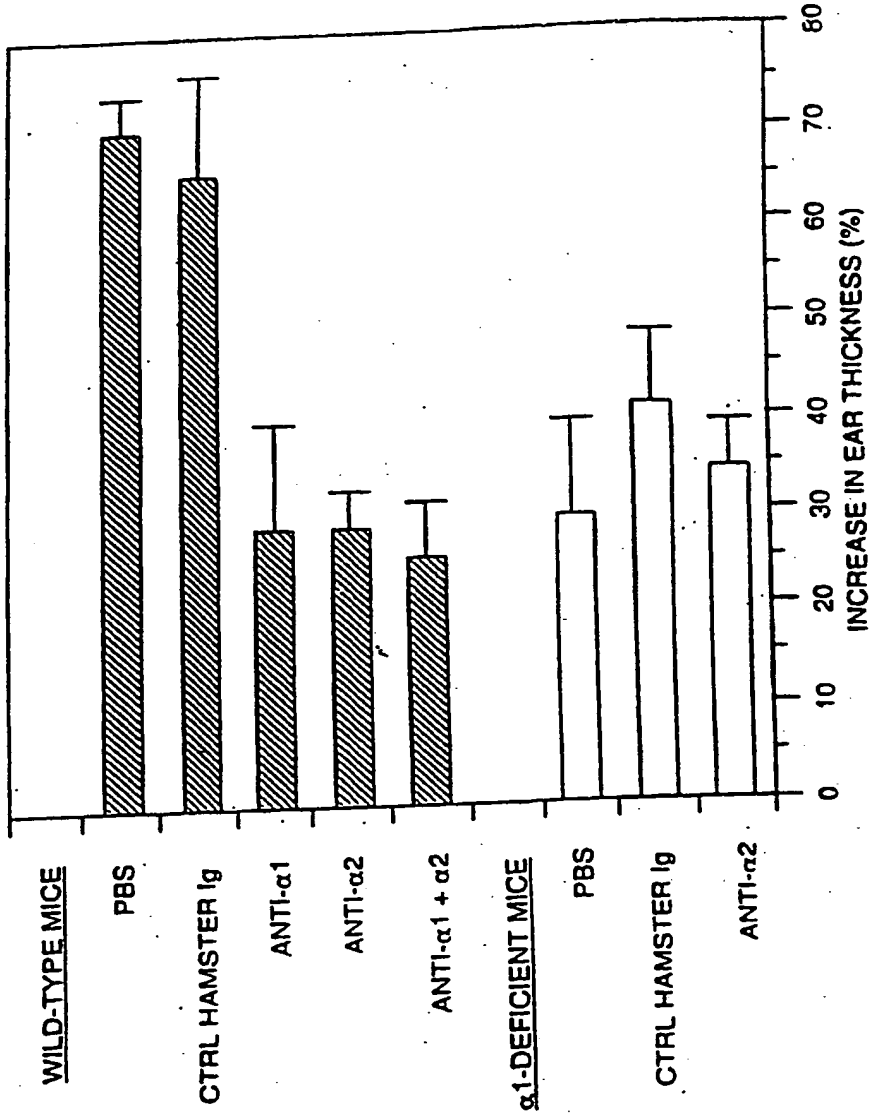

INCREASE IN EAR THICKNESS (%)
0
10
20
30
40
50
60
70
80
WILD-TYPE MICE
PBS
CTRL HAMSTER Ig
ANTI-α1
ANTI-α2
ANTI-α1 + α2
α1-DEFICIENT MICE
PBS
CTRL HAMSTER Ig
ANTI-α2

FIG. 4

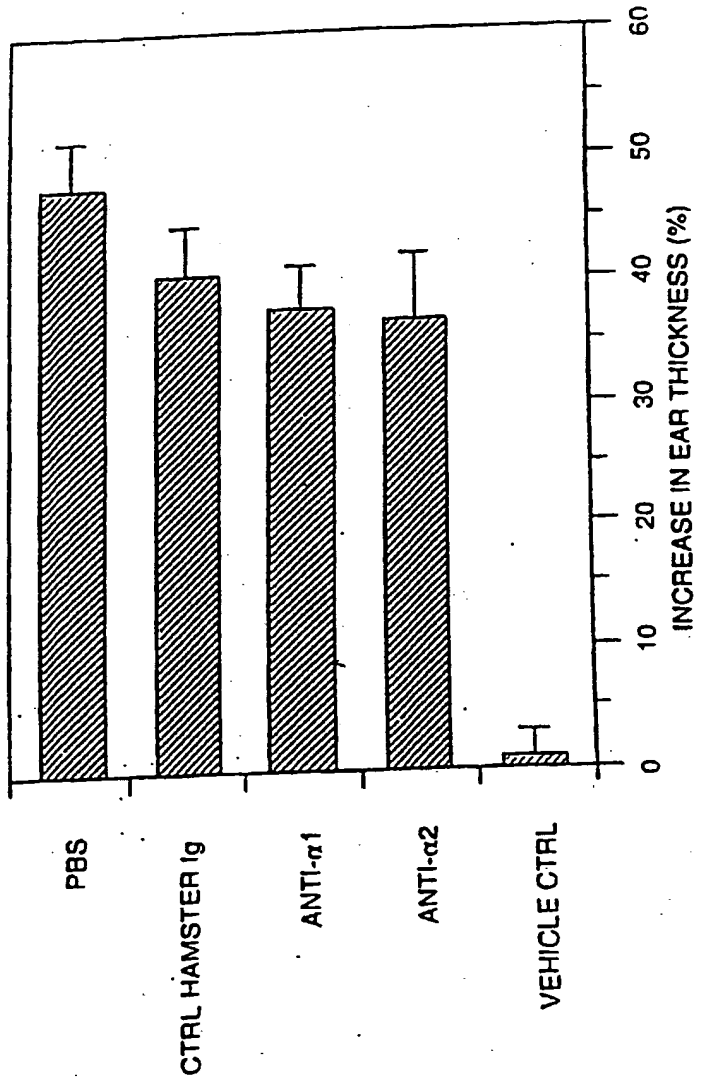

INCREASE IN EAR THICKNESS (%)
0
10
20
30
40
50
60
PBS
CTRL HAMSTER Ig
ANTI-α1
ANTI-α2
VEHICLE CTRL

FIG. 5

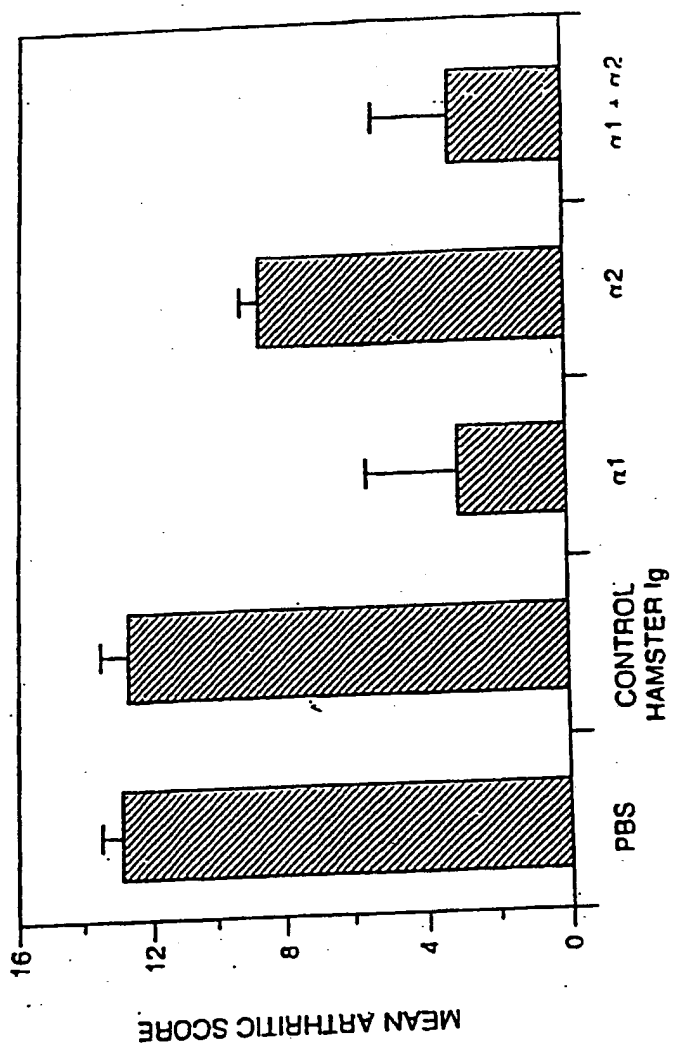

MEAN ARTHRITIC SCORE
16
12
8
4
0
PBS
CONTROL HAMSTER Ig
α1
α2
α1 + α2
mAh TREATMENT

FIG. 6

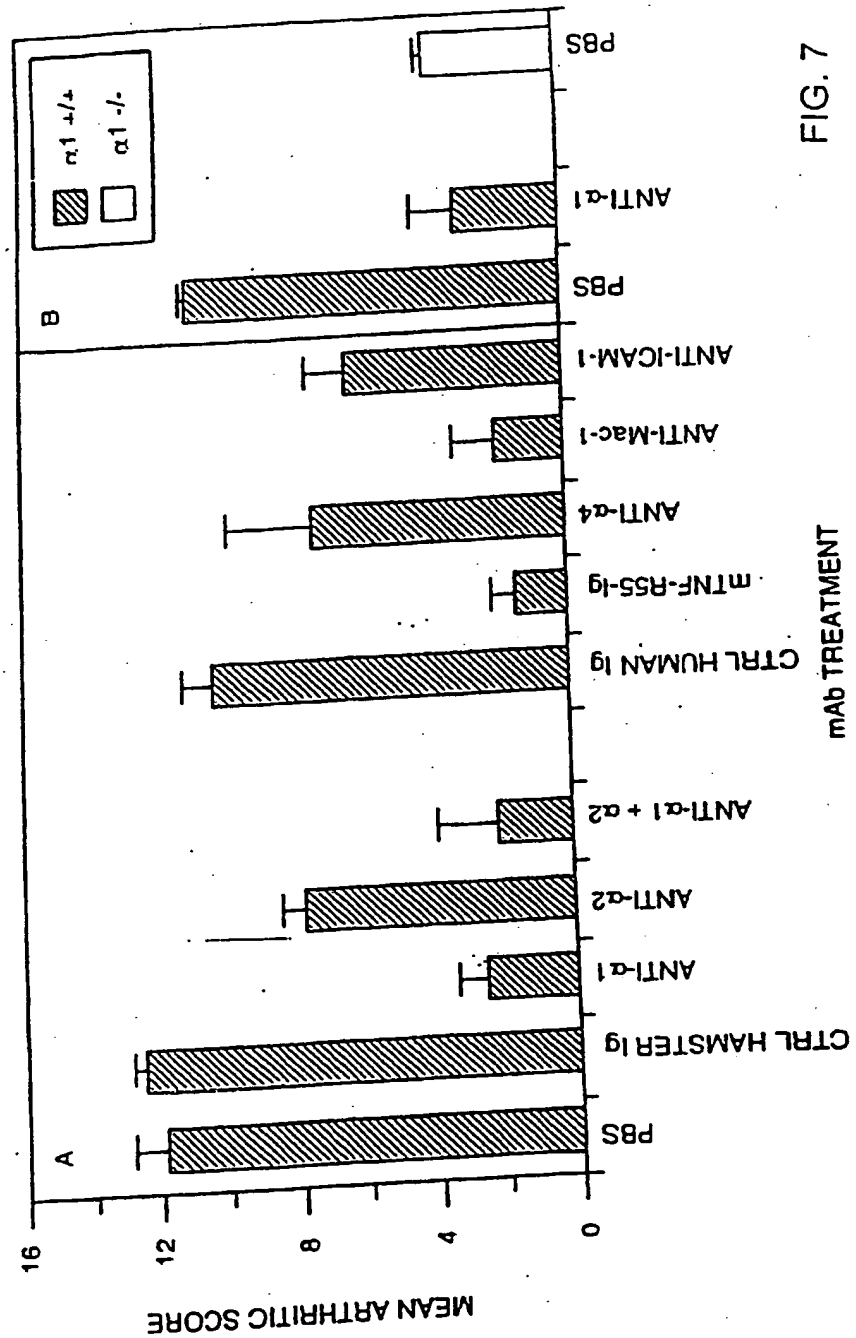

MEAN ARTHRITIC SCORE
16
12
8
4
0
A
B
α1 +/+
α1 -/-
PBS
CTRL HAMSTER Ig
ANTI-α1
ANTI-α2
ANTI-α1 + α2
CTRL HUMAN Ig
mTNF-R55-Ig
ANTI-α4
ANTI-Mac-1
ANTI-ICAM-1
PBS
ANTI-α1
mAb TREATMENT

FIG. 7

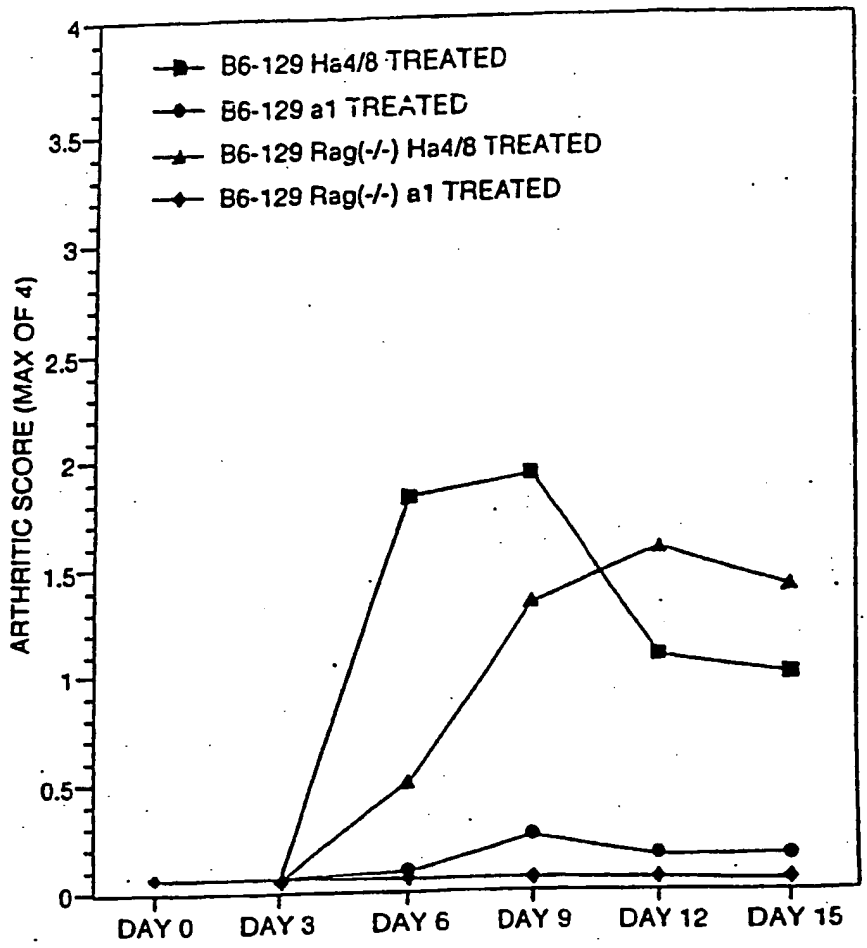

B6-129 Ha4/8 TREATED
B6-129 a1 TREATED
B6-129 Rag(-/-) Ha4/8 TREATED
B6-129 Rag(-/-) a1 TREATED
ARTHRITIC SCORE (MAX OF 4)
4
3.5
3
2.5
2
1.5
1
0.5
0
DAY 0
DAY 3
DAY 6
DAY 9
DAY 12
DAY 15

FIG. 8

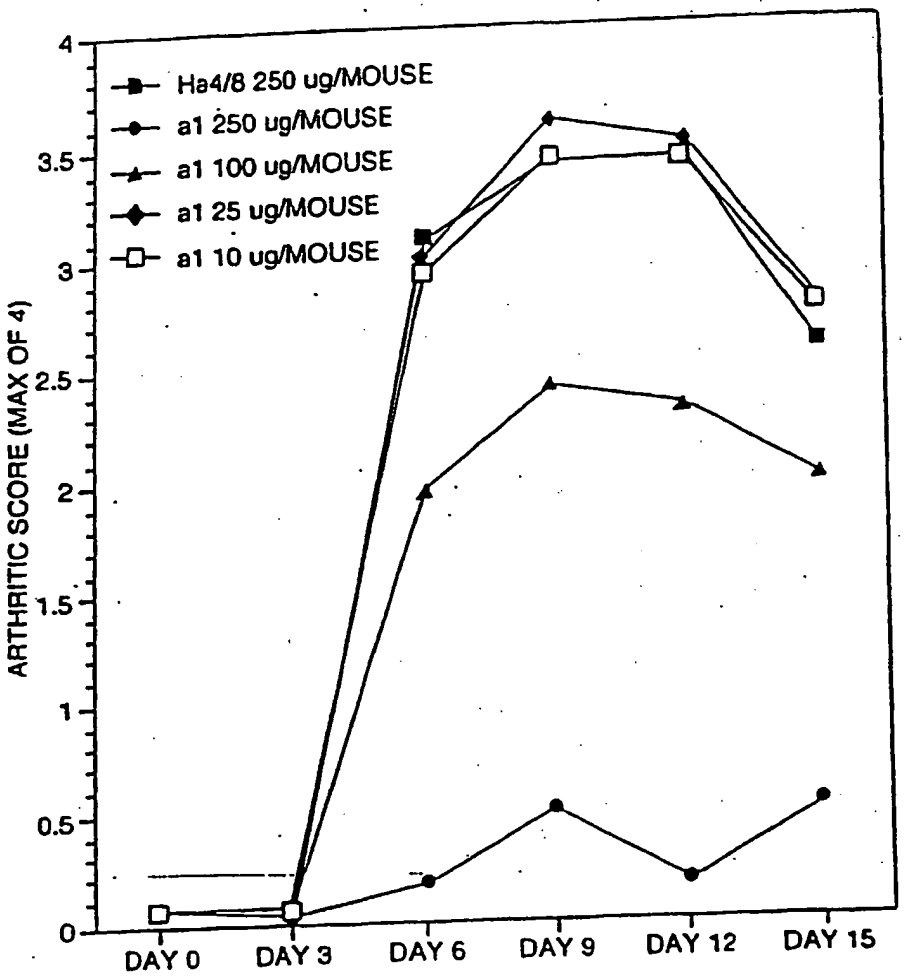

Ha4/8 250 ug/MOUSE
a1 250 ug/MOUSE
a1 100 ug/MOUSE
a1 25 ug/MOUSE
a1 10 ug/MOUSE
ARTHRITIC SCORE (MAX OF 4)
0
0.5
1
1.5
2
2.5
3
3.5
4
DAY 0
DAY 3
DAY 6
DAY 9
DAY 12
DAY 15

FIG. 9

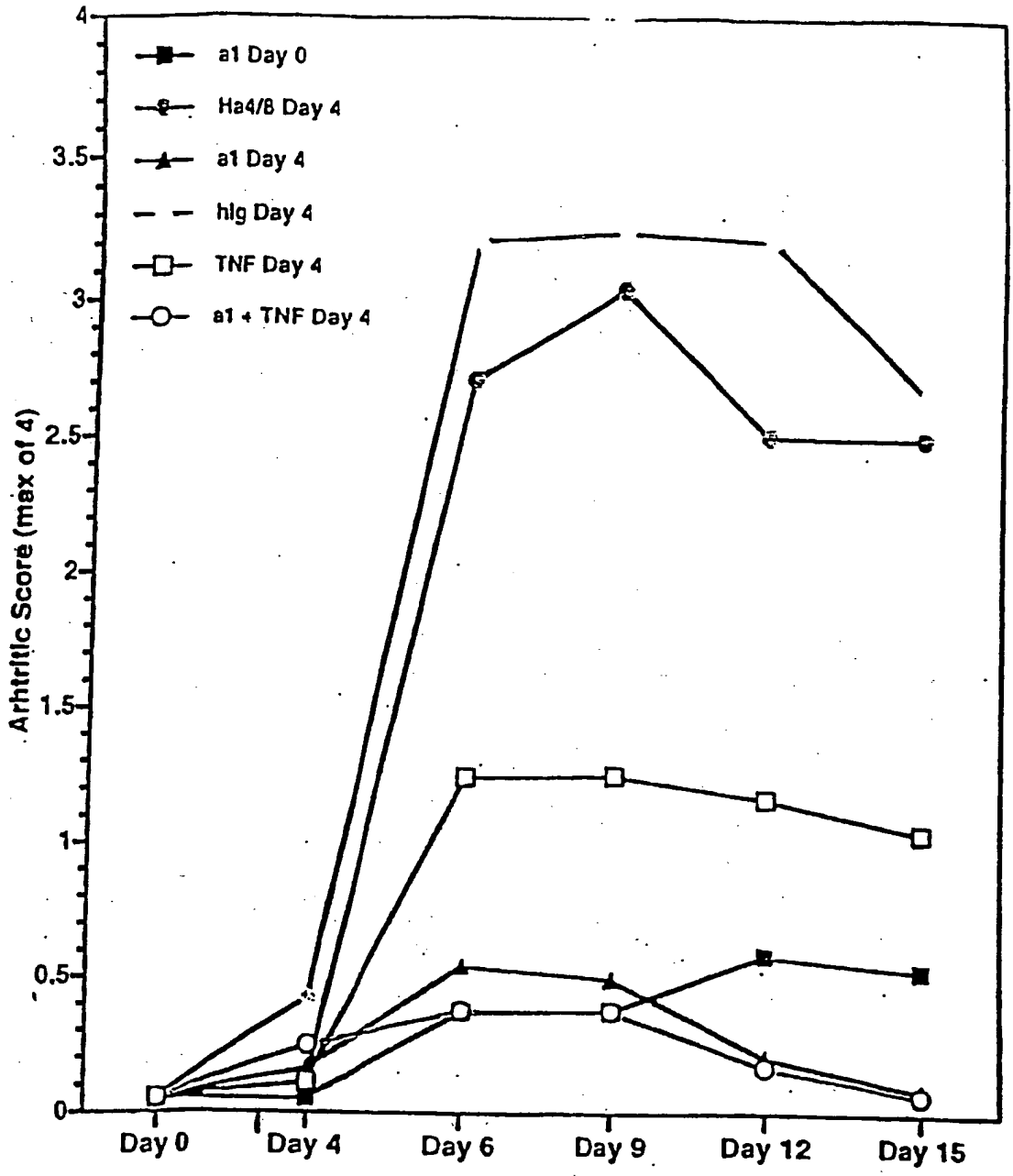

a1 Day 0
Ha4/8 Day 4
a1 Day 4
hIg Day 4
TNF Day 4
a1 + TNF Day 4
Arthritic Score (max of 4)
0
0.5
1
1.5
2
2.5
3
3.5
4
Day 0
Day 4
Day 6
Day 9
Day 12
Day 15

FIG. 10

```
1   V S P T F Q V V N S F A P V Q E C S T C
                      J
21  L D I V I V L D G S N S I Y P W E S V I
                                T       -
41  A F L N D L L K R M D I G P K C T C V G
61  I V Q Y G E N V T H E F N L N K Y S S T
81  E E V L V A A K K I G R Q G G L C T M T
                      V Q R G G R
101 A L G I D T A R K E A F T E A R G A R R
                T
121 G V K K V M V I V T D G E S H D N Y R L
                                  H
141 K Q V I Q D C E D E N I Q R F S I A I L
      K
161 G H Y N R G N L S T E K F V E E I K S I
      S
181 A S E P T E K H F F N V S D E L A L V T
201 I V K A L G E R I F A L E A
        T
```

FIG. 11A

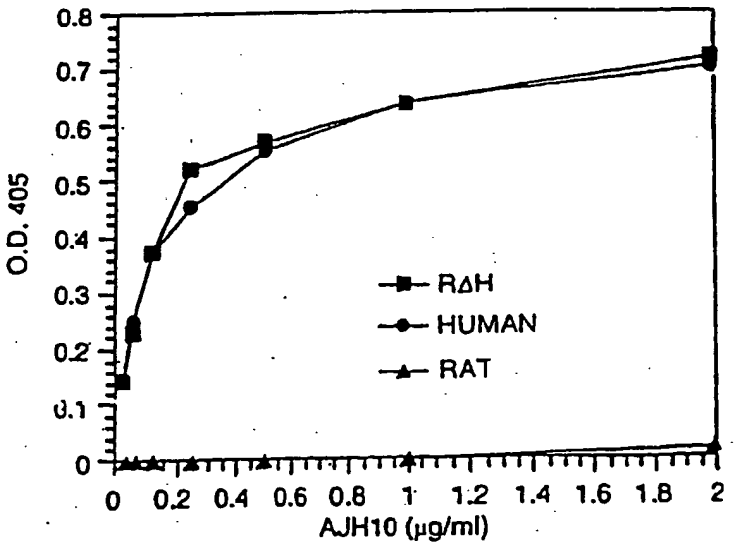



FIG. 11B

```
1   V S P T F Q V V N S I A P V Q E C S T Q
21  L D I V I V L D G S N S I Y P W D S V T
41  A F L N D L L K R M D I G P K Q T Q V G
61  I V Q Y G E N V T H E F N L N K Y S S T
81  E E V L V A A K K I V Q R G G R Q T M T
101 A L G T D T A R K E A F T E A R G A R R
121 G V K K V M V I V T D G E S H D N H R L
141 K K V I Q D C E D E N I Q R F S I A I L
161 G S Y N R G N L S T E K F V E E I K S I
181 A S E P T E K H R F N V S D E L A L V T
201 I V K T L G E R I F A L E A
```

FIG. 12

FIG. 13A

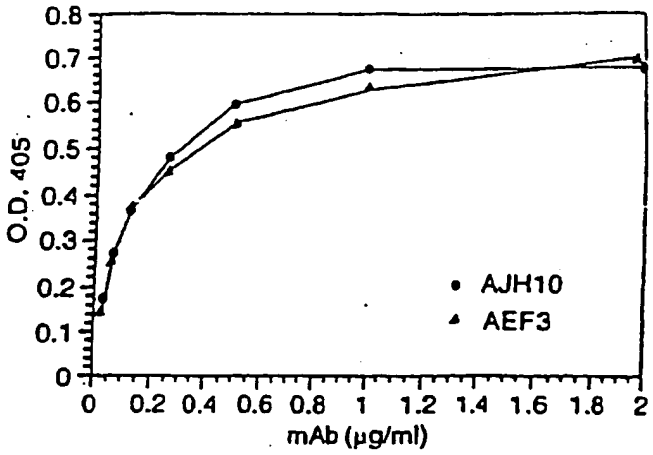



FIG. 13B

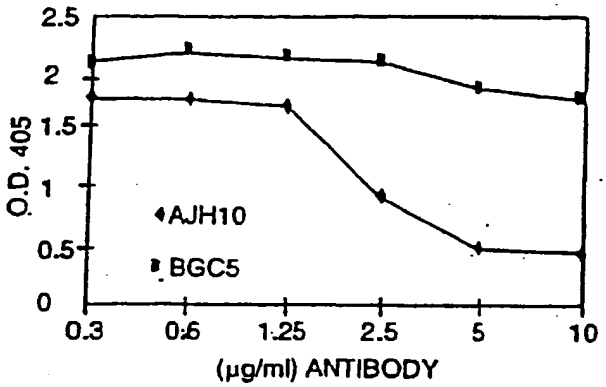
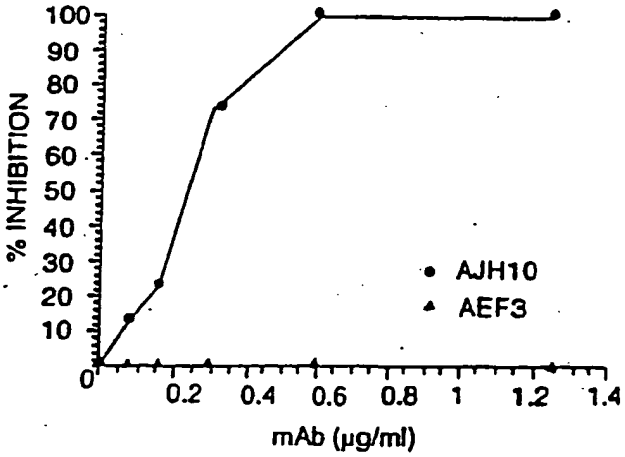



FIG. 13C



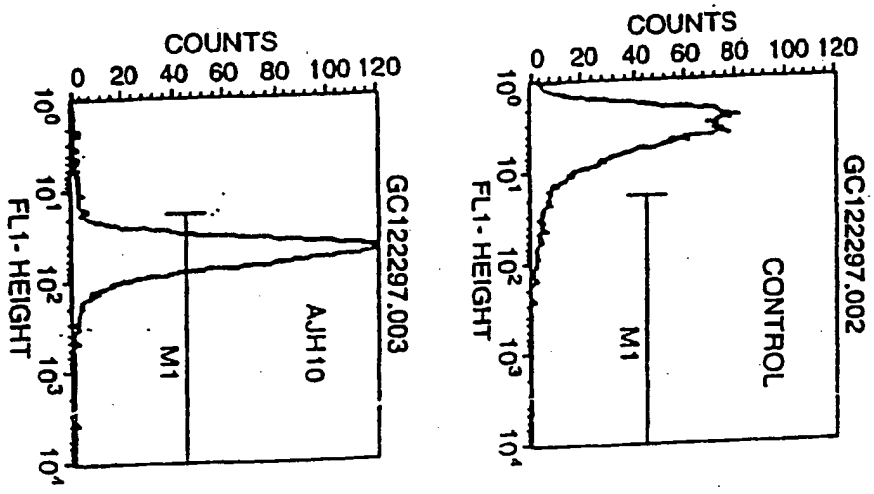

COUNTS
0 20 40 60 80 100 120
FL1-HEIGHT
$10^0$ $10^1$ $10^2$ $10^3$ $10^4$
M1
AJH10
GC122297.003
COUNTS
0 20 40 60 80 100 120
FL1-HEIGHT
$10^0$ $10^1$ $10^2$ $10^3$ $10^4$
M1
CONTROL
GC122297.002

FIG. 14

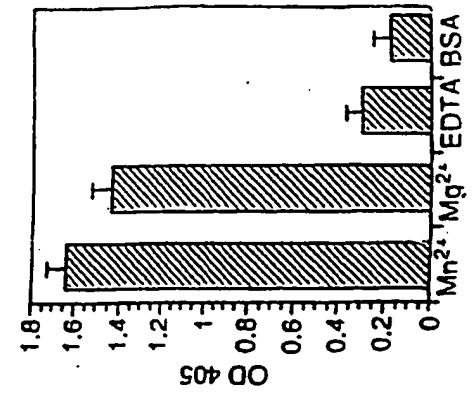



FIG. 15C

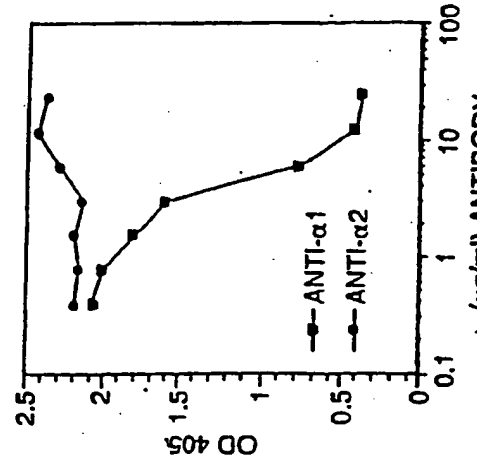



FIG. 15B

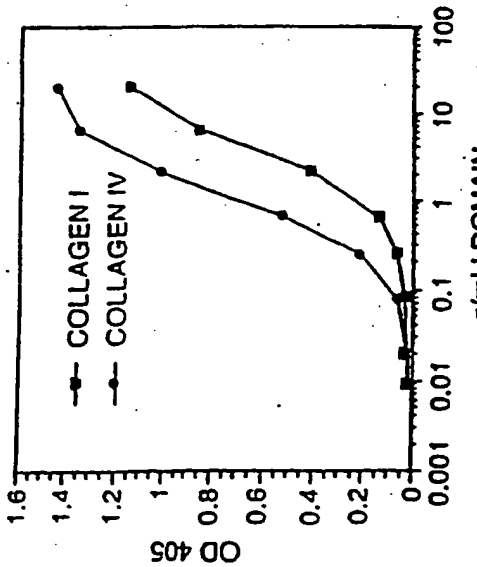
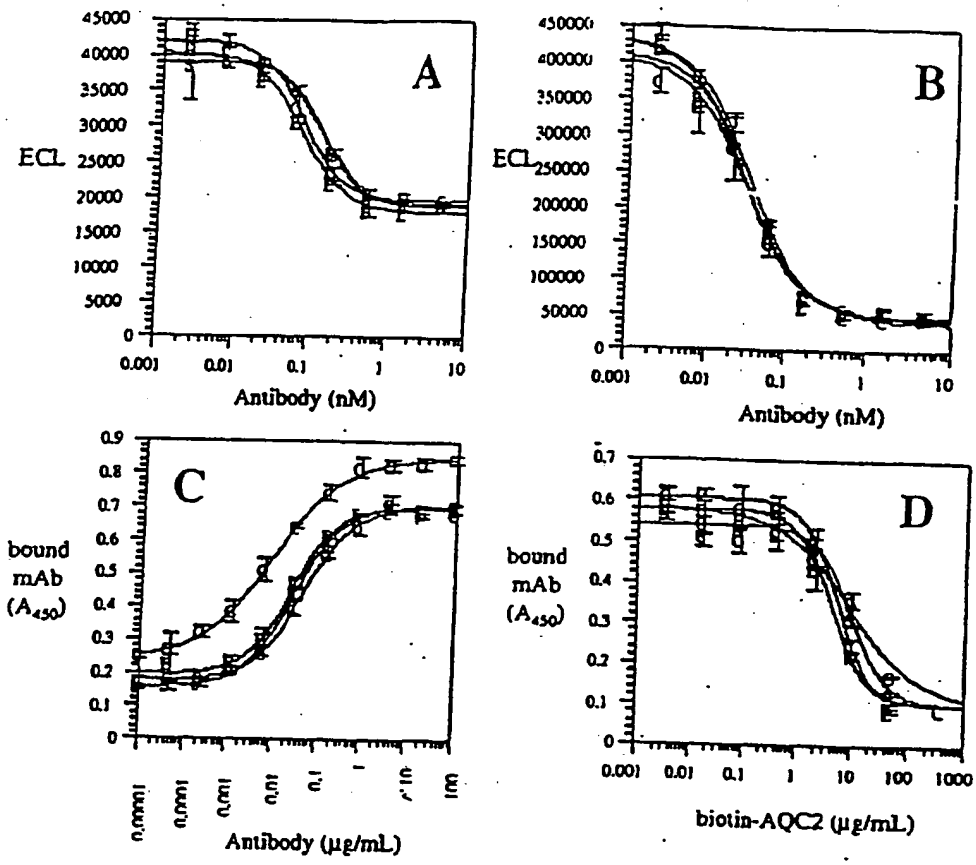
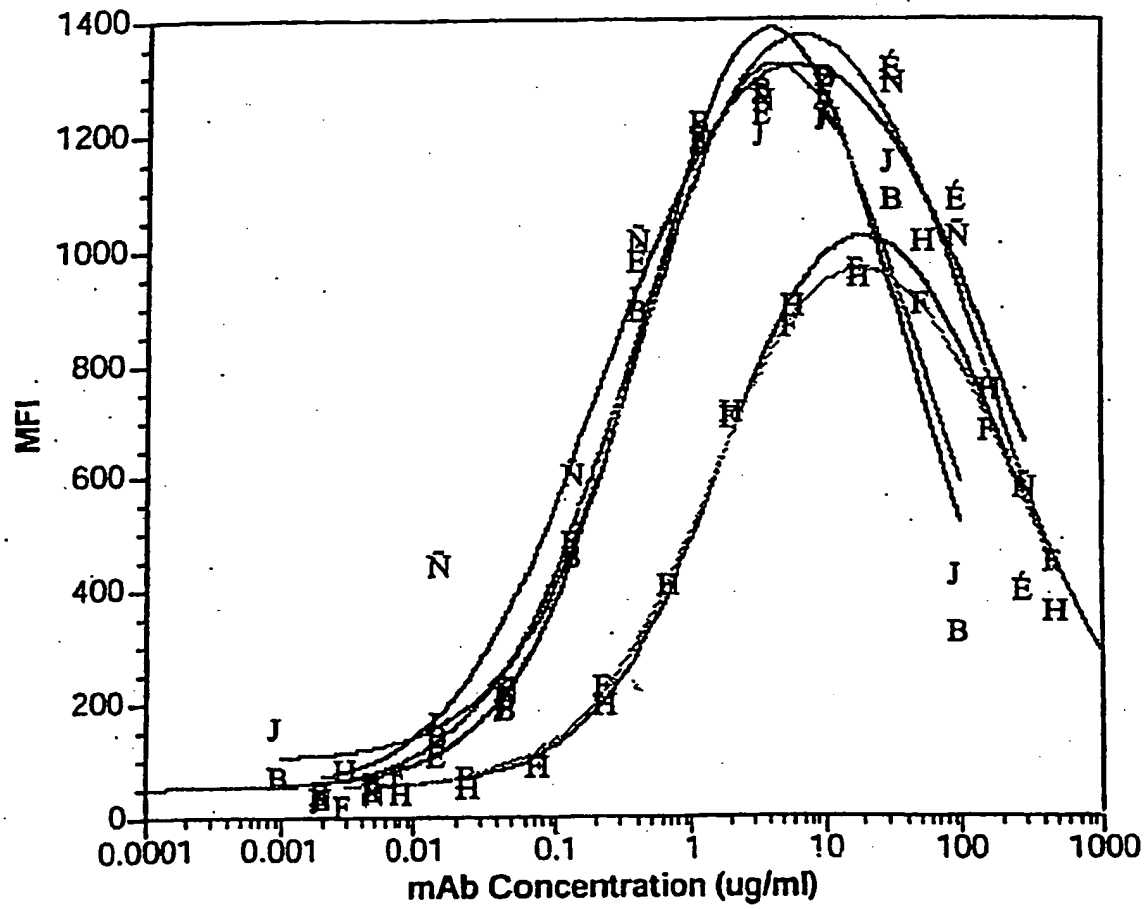



FIG. 15A


A
ECL
Antibody (nM)
B
ECL
Antibody (nM)
C
bound mAb ($A_{450}$)
Antibody (µg/mL)
D
bound mAb ($A_{450}$)
biotin-AQC2 (µg/mL)

FIGS. 16 A, B, C, D

Humanized AQ.C2 Antibodies tested by FACS on K562 α 1 cells




| | |
|---|---|
| B | Consensus 1 |
| J | Homology 1 |
| H | Consensus 2 |
| F | Homology 2 |
| Ñ | Chimeric ACQ2 Blocked |
| É | Chimeric ACQ2 Unblocked |

FIG. 17

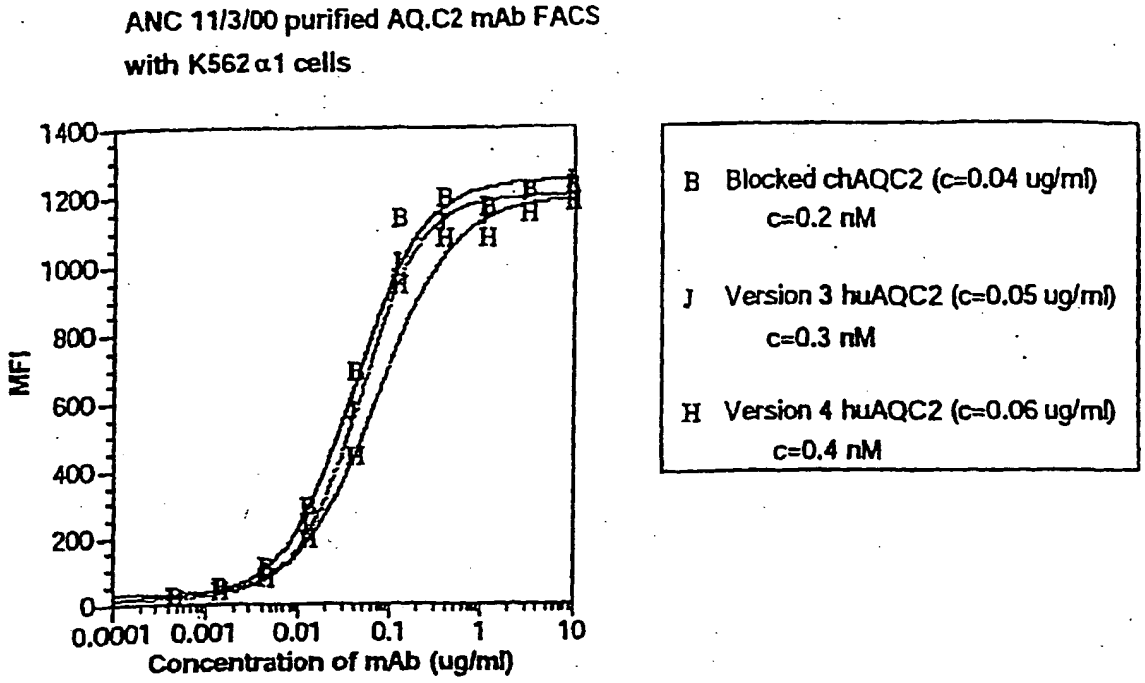

ANC 11/3/00 purified AQ.C2 mAb FACS
with K562 α1 cells
MFI
1400
1200
1000
800
600
400
200
0
0.0001
0.001
0.01
0.1
1
10
Concentration of mAb (ug/ml)
B Blocked chAQC2 (c=0.04 ug/ml)
c=0.2 nM
J Version 3 huAQC2 (c=0.05 ug/ml)
c=0.3 nM
H Version 4 huAQC2 (c=0.06 ug/ml)
c=0.4 nM

FIG. 18

# Fig. 19: A-1

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1 | CB | THR | 145 | 131.250 | 52.244 | -9.297 | 1.00 | 82.68 | A | C |
| ATOM | 2 | OG1 | THR | 145 | 131.373 | 51.127 | -10.191 | 1.00 | 82.68 | A | O |
| ATOM | 3 | CG2 | THR | 145 | 132.601 | 52.936 | -9.145 | 1.00 | 82.68 | A | C |
| ATOM | 4 | C | THR | 145 | 129.280 | 51.301 | -8.080 | 1.00 | 146.54 | A | C |
| ATOM | 5 | O | THR | 145 | 128.489 | 51.352 | -7.134 | 1.00 | 146.94 | A | O |
| ATOM | 6 | N | THR | 145 | 131.576 | 50.663 | -7.360 | 1.00 | 144.92 | A | N |
| ATOM | 7 | CA | THR | 145 | 130.726 | 51.757 | -7.915 | 1.00 | 144.52 | A | C |
| ATOM | 8 | N | GLN | 146 | 128.941 | 50.856 | -9.288 | 1.00 | 36.14 | A | N |
| ATOM | 9 | CA | GLN | 146 | 127.592 | 50.397 | -9.569 | 1.00 | 34.29 | A | C |
| ATOM | 10 | CB | GLN | 146 | 127.046 | 51.086 | -10.823 | 1.00 | 99.89 | A | C |
| ATOM | 11 | CG | GLN | 146 | 127.887 | 50.902 | -12.065 | 1.00 | 99.89 | A | C |
| ATOM | 12 | CD | GLN | 146 | 127.274 | 51.575 | -13.279 | 1.00 | 99.89 | A | C |
| ATOM | 13 | OE1 | GLN | 146 | 127.787 | 51.454 | -14.392 | 1.00 | 99.89 | A | O |
| ATOM | 14 | NE2 | GLN | 146 | 126.170 | 52.290 | -13.070 | 1.00 | 99.89 | A | N |
| ATOM | 15 | C | GLN | 146 | 127.535 | 48.883 | -9.721 | 1.00 | 34.71 | A | C |
| ATOM | 16 | O | GLN | 146 | 128.084 | 48.314 | -10.667 | 1.00 | 36.57 | A | O |
| ATOM | 17 | N | LEU | 147 | 126.876 | 48.240 | -8.762 | 1.00 | 33.54 | A | N |
| ATOM | 18 | CA | LEU | 147 | 126.718 | 46.794 | -8.767 | 1.00 | 32.67 | A | C |
| ATOM | 19 | CB | LEU | 147 | 127.491 | 46.143 | -7.609 | 1.00 | 35.25 | A | C |
| ATOM | 20 | CG | LEU | 147 | 128.963 | 46.398 | -7.301 | 1.00 | 35.44 | A | C |
| ATOM | 21 | CD1 | LEU | 147 | 129.205 | 47.877 | -7.087 | 1.00 | 30.65 | A | C |
| ATOM | 22 | CD2 | LEU | 147 | 129.325 | 45.637 | -6.037 | 1.00 | 35.29 | A | C |
| ATOM | 23 | C | LEU | 147 | 125.247 | 46.451 | -8.575 | 1.00 | 31.65 | A | C |
| ATOM | 24 | O | LEU | 147 | 124.506 | 47.194 | -7.939 | 1.00 | 32.95 | A | O |
| ATOM | 25 | N | ASP | 148 | 124.832 | 45.325 | -9.142 | 1.00 | 25.19 | A | N |
| ATOM | 26 | CA | ASP | 148 | 123.477 | 44.817 | -8.976 | 1.00 | 22.65 | A | C |
| ATOM | 27 | CB | ASP | 148 | 122.907 | 44.329 | -10.302 | 1.00 | 27.55 | A | C |
| ATOM | 28 | CG | ASP | 148 | 122.330 | 45.446 | -11.125 | 1.00 | 27.17 | A | C |
| ATOM | 29 | OD1 | ASP | 148 | 121.787 | 45.158 | -12.208 | 1.00 | 26.28 | A | O |
| ATOM | 30 | OD2 | ASP | 148 | 122.413 | 46.612 | -10.686 | 1.00 | 25.35 | A | O |
| ATOM | 31 | C | ASP | 148 | 123.664 | 43.638 | -8.025 | 1.00 | 19.03 | A | C |
| ATOM | 32 | O | ASP | 148 | 124.119 | 42.567 | -8.422 | 1.00 | 18.33 | A | O |
| ATOM | 33 | N | ILE | 149 | 123.341 | 43.848 | -6.760 | 1.00 | 16.75 | A | N |
| ATOM | 34 | CA | ILE | 149 | 123.502 | 42.809 | -5.761 | 1.00 | 15.69 | A | C |
| ATOM | 35 | CB | ILE | 149 | 124.041 | 43.391 | -4.442 | 1.00 | 18.53 | A | C |
| ATOM | 36 | CG2 | ILE | 149 | 124.401 | 42.269 | -3.485 | 1.00 | 13.54 | A | C |
| ATOM | 37 | CG1 | ILE | 149 | 125.271 | 44.251 | -4.718 | 1.00 | 14.25 | A | C |
| ATOM | 38 | CD1 | ILE | 149 | 125.819 | 44.932 | -3.497 | 1.00 | 17.00 | A | C |
| ATOM | 39 | C | ILE | 149 | 122.185 | 42.129 | -5.456 | 1.00 | 17.34 | A | C |
| ATOM | 40 | O | ILE | 149 | 121.191 | 42.794 | -5.181 | 1.00 | 17.74 | A | O |
| ATOM | 41 | N | VAL | 150 | 122.175 | 40.805 | -5.526 | 1.00 | 11.00 | A | N |
| ATOM | 42 | CA | VAL | 150 | 120.987 | 40.036 | -5.193 | 1.00 | 12.56 | A | C |
| ATOM | 43 | CB | VAL | 150 | 120.571 | 39.089 | -6.336 | 1.00 | 16.85 | A | C |
| ATOM | 44 | CG1 | VAL | 150 | 119.409 | 38.210 | -5.885 | 1.00 | 19.04 | A | C |
| ATOM | 45 | CG2 | VAL | 150 | 120.164 | 39.894 | -7.555 | 1.00 | 18.66 | A | C |
| ATOM | 46 | C | VAL | 150 | 121.367 | 39.212 | -3.970 | 1.00 | 10.12 | A | C |
| ATOM | 47 | O | VAL | 150 | 122.387 | 38.526 | -3.973 | 1.00 | 8.27 | A | O |
| ATOM | 48 | N | ILE | 151 | 120.573 | 39.303 | -2.912 | 1.00 | 20.50 | A | N |
| ATOM | 49 | CA | ILE | 151 | 120.856 | 38.537 | -1.699 | 1.00 | 19.30 | A | C |
| ATOM | 50 | CB | ILE | 151 | 120.653 | 39.392 | -0.439 | 1.00 | 14.22 | A | C |
| ATOM | 51 | CG2 | ILE | 151 | 121.039 | 38.601 | 0.785 | 1.00 | 10.58 | A | C |
| ATOM | 52 | CG1 | ILE | 151 | 121.515 | 40.659 | -0.532 | 1.00 | 12.64 | A | C |
| ATOM | 53 | CD1 | ILE | 151 | 121.283 | 41.660 | 0.593 | 1.00 | 14.62 | A | C |
| ATOM | 54 | C | ILE | 151 | 119.931 | 37.329 | -1.646 | 1.00 | 17.42 | A | C |
| ATOM | 55 | O | ILE | 151 | 118.715 | 37.459 | -1.777 | 1.00 | 17.66 | A | O |
| ATOM | 56 | N | VAL | 152 | 120.511 | 36.150 | -1.470 | 1.00 | 17.56 | A | N |
| ATOM | 57 | CA | VAL | 152 | 119.741 | 34.915 | -1.428 | 1.00 | 18.41 | A | C |
| ATOM | 58 | CB | VAL | 152 | 120.395 | 33.849 | -2.309 | 1.00 | 11.45 | A | C |
| ATOM | 59 | CG1 | VAL | 152 | 119.470 | 32.664 | -2.460 | 1.00 | 10.58 | A | C |
| ATOM | 60 | CG2 | VAL | 152 | 120.758 | 34.458 | -3.667 | 1.00 | 7.89 | A | C |
| ATOM | 61 | C | VAL | 152 | 119.675 | 34.404 | -0.003 | 1.00 | 16.31 | A | C |
| ATOM | 62 | O | VAL | 152 | 120.602 | 33.755 | 0.469 | 1.00 | 9.91 | A | O |
| ATOM | 63 | N | LEU | 153 | 118.568 | 34.692 | 0.672 | 1.00 | 19.79 | A | N |
| ATOM | 64 | CA | LEU | 153 | 118.367 | 34.297 | 2.061 | 1.00 | 19.90 | A | C |
| ATOM | 65 | CB | LEU | 153 | 117.530 | 35.361 | 2.766 | 1.00 | 21.44 | A | C |
| ATOM | 66 | CG | LEU | 153 | 118.250 | 36.403 | 3.623 | 1.00 | 23.22 | A | C |
| ATOM | 67 | CD1 | LEU | 153 | 119.699 | 36.561 | 3.185 | 1.00 | 23.73 | A | C |
| ATOM | 68 | CD2 | LEU | 153 | 117.494 | 37.721 | 3.530 | 1.00 | 25.76 | A | C |
| ATOM | 69 | C | LEU | 153 | 117.732 | 32.929 | 2.300 | 1.00 | 20.96 | A | C |
| ATOM | 70 | O | LEU | 153 | 116.724 | 32.574 | 1.690 | 1.00 | 19.96 | A | O |
| ATOM | 71 | N | ASP | 154 | 118.336 | 32.165 | 3.200 | 1.00 | 19.89 | A | N |
| ATOM | 72 | CA | ASP | 154 | 117.820 | 30.854 | 3.554 | 1.00 | 19.37 | A | C |
| ATOM | 73 | CB | ASP | 154 | 118.952 | 29.983 | 4.129 | 1.00 | 22.72 | A | C |

Fig. 19: A-2

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 74 | CG | ASP | 154 | 118.486 | 28.601 | 4.546 | 1.00 | 21.92 | A | C |
| ATOM | 75 | OD1 | ASP | 154 | 117.266 | 28.363 | 4.537 | 1.00 | 25.43 | A | O |
| ATOM | 76 | OD2 | ASP | 154 | 119.340 | 27.754 | 4.893 | 1.00 | 18.24 | A | O |
| ATOM | 77 | C | ASP | 154 | 116.770 | 31.153 | 4.623 | 1.00 | 22.71 | A | C |
| ATOM | 78 | O | ASP | 154 | 117.062 | 31.802 | 5.630 | 1.00 | 19.03 | A | O |
| ATOM | 79 | N | GLY | 155 | 115.540 | 30.718 | 4.393 | 1.00 | 3.06 | A | N |
| ATOM | 80 | CA | GLY | 155 | 114.491 | 30.948 | 5.370 | 1.00 | 5.13 | A | C |
| ATOM | 81 | C | GLY | 155 | 113.840 | 29.638 | 5.788 | 1.00 | 6.39 | A | C |
| ATOM | 82 | O | GLY | 155 | 112.751 | 29.633 | 6.368 | 1.00 | 8.88 | A | O |
| ATOM | 83 | N | SER | 156 | 114.512 | 28.521 | 5.494 | 1.00 | 19.70 | A | N |
| ATOM | 84 | CA | SER | 156 | 114.011 | 27.191 | 5.832 | 1.00 | 24.28 | A | C |
| ATOM | 85 | CB | SER | 156 | 114.994 | 26.111 | 5.353 | 1.00 | 33.45 | A | C |
| ATOM | 86 | OG | SER | 156 | 116.261 | 26.252 | 5.967 | 1.00 | 36.37 | A | O |
| ATOM | 87 | C | SER | 156 | 113.773 | 27.054 | 7.330 | 1.00 | 21.27 | A | C |
| ATOM | 88 | O | SER | 156 | 114.270 | 27.843 | 8.128 | 1.00 | 24.45 | A | O |
| ATOM | 89 | N | ASN | 157 | 113.008 | 26.037 | 7.700 | 1.00 | 21.98 | A | N |
| ATOM | 90 | CA | ASN | 157 | 112.686 | 25.802 | 9.091 | 1.00 | 19.06 | A | C |
| ATOM | 91 | CB | ASN | 157 | 112.027 | 24.435 | 9.247 | 1.00 | 21.82 | A | C |
| ATOM | 92 | CG | ASN | 157 | 110.586 | 24.434 | 8.785 | 1.00 | 23.31 | A | C |
| ATOM | 93 | OD1 | ASN | 157 | 109.944 | 23.385 | 8.706 | 1.00 | 20.38 | A | O |
| ATOM | 94 | ND2 | ASN | 157 | 110.066 | 25.612 | 8.479 | 1.00 | 20.59 | A | N |
| ATOM | 95 | C | ASN | 157 | 113.859 | 25.913 | 10.048 | 1.00 | 17.03 | A | C |
| ATOM | 96 | O | ASN | 157 | 113.720 | 26.498 | 11.132 | 1.00 | 15.01 | A | O |
| ATOM | 97 | N | SER | 158 | 115.006 | 25.367 | 9.653 | 1.00 | 15.99 | A | N |
| ATOM | 98 | CA | SER | 158 | 116.179 | 25.378 | 10.510 | 1.00 | 14.20 | A | C |
| ATOM | 99 | CB | SER | 158 | 117.327 | 24.603 | 9.864 | 1.00 | 26.18 | A | C |
| ATOM | 100 | OG | SER | 158 | 117.597 | 25.067 | 8.562 | 1.00 | 28.89 | A | O |
| ATOM | 101 | C | SER | 158 | 116.656 | 26.753 | 10.941 | 1.00 | 14.97 | A | C |
| ATOM | 102 | O | SER | 158 | 117.053 | 26.930 | 12.097 | 1.00 | 12.14 | A | O |
| ATOM | 103 | N | ILE | 159 | 116.623 | 27.730 | 10.039 | 1.00 | 8.33 | A | N |
| ATOM | 104 | CA | ILE | 159 | 117.050 | 29.083 | 10.379 | 1.00 | 12.93 | A | C |
| ATOM | 105 | CB | ILE | 159 | 116.801 | 30.035 | 9.193 | 1.00 | 9.66 | A | C |
| ATOM | 106 | CG2 | ILE | 159 | 117.138 | 31.479 | 9.592 | 1.00 | 9.57 | A | C |
| ATOM | 107 | CG1 | ILE | 159 | 117.650 | 29.609 | 8.000 | 1.00 | 14.44 | A | C |
| ATOM | 108 | CD1 | ILE | 159 | 119.134 | 29.804 | 8.204 | 1.00 | 19.60 | A | C |
| ATOM | 109 | C | ILE | 159 | 116.292 | 29.604 | 11.616 | 1.00 | 17.24 | A | C |
| ATOM | 110 | O | ILE | 159 | 115.059 | 29.575 | 11.659 | 1.00 | 16.65 | A | O |
| ATOM | 111 | N | TYR | 160 | 117.032 | 30.084 | 12.611 | 1.00 | 29.54 | A | N |
| ATOM | 112 | CA | TYR | 160 | 116.438 | 30.600 | 13.849 | 1.00 | 31.67 | A | C |
| ATOM | 113 | CB | TYR | 160 | 115.775 | 29.455 | 14.639 | 1.00 | 16.89 | A | C |
| ATOM | 114 | CG | TYR | 160 | 115.094 | 29.869 | 15.941 | 1.00 | 13.65 | A | C |
| ATOM | 115 | CD1 | TYR | 160 | 113.717 | 30.089 | 15.993 | 1.00 | 16.07 | A | C |
| ATOM | 116 | CE1 | TYR | 160 | 113.088 | 30.466 | 17.186 | 1.00 | 13.67 | A | C |
| ATOM | 117 | CD2 | TYR | 160 | 115.828 | 30.038 | 17.116 | 1.00 | 11.30 | A | C |
| ATOM | 118 | CE2 | TYR | 160 | 115.211 | 30.416 | 18.304 | 1.00 | 15.01 | A | C |
| ATOM | 119 | CZ | TYR | 160 | 113.841 | 30.627 | 18.338 | 1.00 | 14.36 | A | C |
| ATOM | 120 | OH | TYR | 160 | 113.227 | 30.987 | 19.522 | 1.00 | 19.36 | A | O |
| ATOM | 121 | C | TYR | 160 | 117.498 | 31.264 | 14.734 | 1.00 | 33.39 | A | C |
| ATOM | 122 | O | TYR | 160 | 118.567 | 30.703 | 14.970 | 1.00 | 39.31 | A | O |
| ATOM | 123 | N | PRO | 161 | 117.206 | 32.467 | 15.248 | 1.00 | 31.87 | A | N |
| ATOM | 124 | CD | PRO | 161 | 117.988 | 33.002 | 16.380 | 1.00 | 14.17 | A | C |
| ATOM | 125 | CA | PRO | 161 | 115.969 | 33.234 | 15.055 | 1.00 | 30.15 | A | C |
| ATOM | 126 | CB | PRO | 161 | 115.831 | 33.976 | 16.379 | 1.00 | 18.55 | A | C |
| ATOM | 127 | CG | PRO | 161 | 117.278 | 34.291 | 16.703 | 1.00 | 21.71 | A | C |
| ATOM | 128 | C | PRO | 161 | 116.038 | 34.183 | 13.852 | 1.00 | 28.81 | A | C |
| ATOM | 129 | O | PRO | 161 | 117.074 | 34.792 | 13.580 | 1.00 | 28.13 | A | O |
| ATOM | 130 | N | TRP | 162 | 114.919 | 34.320 | 13.149 | 1.00 | 29.23 | A | N |
| ATOM | 131 | CA | TRP | 162 | 114.839 | 35.170 | 11.967 | 1.00 | 30.30 | A | C |
| ATOM | 132 | CB | TRP | 162 | 113.388 | 35.250 | 11.493 | 1.00 | 29.17 | A | C |
| ATOM | 133 | CG | TRP | 162 | 113.214 | 35.826 | 10.120 | 1.00 | 29.69 | A | C |
| ATOM | 134 | CD2 | TRP | 162 | 113.838 | 35.375 | 8.912 | 1.00 | 24.53 | A | C |
| ATOM | 135 | CE2 | TRP | 162 | 113.338 | 36.175 | 7.859 | 1.00 | 28.08 | A | C |
| ATOM | 136 | CE3 | TRP | 162 | 114.768 | 34.373 | 8.615 | 1.00 | 23.94 | A | C |
| ATOM | 137 | CD1 | TRP | 162 | 112.387 | 36.854 | 9.758 | 1.00 | 28.88 | A | C |
| ATOM | 138 | NE1 | TRP | 162 | 112.455 | 37.071 | 8.403 | 1.00 | 30.75 | A | N |
| ATOM | 139 | CZ2 | TRP | 162 | 113.741 | 36.000 | 6.532 | 1.00 | 26.62 | A | C |
| ATOM | 140 | CZ3 | TRP | 162 | 115.167 | 34.202 | 7.288 | 1.00 | 22.27 | A | C |
| ATOM | 141 | CH2 | TRP | 162 | 114.652 | 35.012 | 6.268 | 1.00 | 27.18 | A | C |
| ATOM | 142 | C | TRP | 162 | 115.381 | 36.579 | 12.210 | 1.00 | 32.08 | A | C |
| ATOM | 143 | O | TRP | 162 | 116.074 | 37.133 | 11.352 | 1.00 | 31.23 | A | O |
| ATOM | 144 | N | GLU | 163 | 115.077 | 37.147 | 13.381 | 1.00 | 25.22 | A | N |
| ATOM | 145 | CA | GLU | 163 | 115.510 | 38.504 | 13.734 | 1.00 | 27.00 | A | C |
| ATOM | 146 | CB | GLU | 163 | 115.108 | 38.857 | 15.172 | 1.00 | 105.95 | A | C |

# Fig. 19: A-3

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 147 | CG | GLU | 163 | 115.906 | 38.145 | 16.248 | 1.00 | 112.26 | A | C |
| ATOM | 148 | CD | GLU | 163 | 115.816 | 38.833 | 17.603 | 1.00 | 114.40 | A | C |
| ATOM | 149 | OE1 | GLU | 163 | 116.310 | 39.975 | 17.732 | 1.00 | 116.11 | A | O |
| ATOM | 150 | OE2 | GLU | 163 | 115.253 | 38.232 | 18.541 | 1.00 | 113.36 | A | O |
| ATOM | 151 | C | GLU | 163 | 117.008 | 38.723 | 13.557 | 1.00 | 26.66 | A | C |
| ATOM | 152 | O | GLU | 163 | 117.448 | 39.799 | 13.136 | 1.00 | 22.83 | A | O |
| ATOM | 153 | N | SER | 164 | 117.800 | 37.709 | 13.865 | 1.00 | 20.71 | A | N |
| ATOM | 154 | CA | SER | 164 | 119.241 | 37.850 | 13.715 | 1.00 | 17.90 | A | C |
| ATOM | 155 | CB | SER | 164 | 119.955 | 36.647 | 14.335 | 1.00 | 27.61 | A | C |
| ATOM | 156 | OG | SER | 164 | 119.716 | 36.582 | 15.731 | 1.00 | 33.50 | A | O |
| ATOM | 157 | C | SER | 164 | 119.601 | 37.988 | 12.235 | 1.00 | 18.66 | A | C |
| ATOM | 158 | O | SER | 164 | 120.436 | 38.813 | 11.863 | 1.00 | 21.86 | A | O |
| ATOM | 159 | N | VAL | 165 | 118.956 | 37.179 | 11.398 | 1.00 | 9.03 | A | N |
| ATOM | 160 | CA | VAL | 165 | 119.189 | 37.213 | 9.961 | 1.00 | 8.42 | A | C |
| ATOM | 161 | CB | VAL | 165 | 118.303 | 36.166 | 9.226 | 1.00 | 21.53 | A | C |
| ATOM | 162 | CG1 | VAL | 165 | 118.296 | 36.430 | 7.721 | 1.00 | 22.92 | A | C |
| ATOM | 163 | CG2 | VAL | 165 | 118.826 | 34.760 | 9.505 | 1.00 | 24.53 | A | C |
| ATOM | 164 | C | VAL | 165 | 118.873 | 38.595 | 9.411 | 1.00 | 9.58 | A | C |
| ATOM | 165 | O | VAL | 165 | 119.610 | 39.131 | 8.574 | 1.00 | 11.40 | A | O |
| ATOM | 166 | N | ILE | 166 | 117.772 | 39.169 | 9.887 | 1.00 | 17.73 | A | N |
| ATOM | 167 | CA | ILE | 166 | 117.351 | 40.482 | 9.427 | 1.00 | 17.05 | A | C |
| ATOM | 168 | CB | ILE | 166 | 115.903 | 40.763 | 9.840 | 1.00 | 21.02 | A | C |
| ATOM | 169 | CG2 | ILE | 166 | 115.489 | 42.162 | 9.413 | 1.00 | 20.23 | A | C |
| ATOM | 170 | CG1 | ILE | 166 | 114.997 | 39.737 | 9.164 | 1.00 | 20.88 | A | C |
| ATOM | 171 | CD1 | ILE | 166 | 113.538 | 39.919 | 9.499 | 1.00 | 17.28 | A | C |
| ATOM | 172 | C | ILE | 166 | 118.281 | 41.564 | 9.929 | 1.00 | 16.50 | A | C |
| ATOM | 173 | O | ILE | 166 | 118.560 | 42.520 | 9.206 | 1.00 | 18.25 | A | O |
| ATOM | 174 | N | ALA | 167 | 118.774 | 41.413 | 11.157 | 1.00 | 25.46 | A | N |
| ATOM | 175 | CA | ALA | 167 | 119.711 | 42.391 | 11.710 | 1.00 | 26.06 | A | C |
| ATOM | 176 | CB | ALA | 167 | 120.095 | 42.021 | 13.100 | 1.00 | 7.73 | A | C |
| ATOM | 177 | C | ALA | 167 | 120.941 | 42.371 | 10.823 | 1.00 | 27.27 | A | C |
| ATOM | 178 | O | ALA | 167 | 121.546 | 43.414 | 10.544 | 1.00 | 23.87 | A | O |
| ATOM | 179 | N | PHE | 168 | 121.303 | 41.167 | 10.383 | 1.00 | 18.13 | A | N |
| ATOM | 180 | CA | PHE | 168 | 122.442 | 40.989 | 9.498 | 1.00 | 16.65 | A | C |
| ATOM | 181 | CB | PHE | 168 | 122.626 | 39.513 | 9.158 | 1.00 | 32.51 | A | C |
| ATOM | 182 | CG | PHE | 168 | 123.514 | 39.273 | 7.970 | 1.00 | 31.01 | A | C |
| ATOM | 183 | CD1 | PHE | 168 | 122.968 | 39.066 | 6.701 | 1.00 | 32.61 | A | C |
| ATOM | 184 | CD2 | PHE | 168 | 124.894 | 39.290 | 8.106 | 1.00 | 29.32 | A | C |
| ATOM | 185 | CE1 | PHE | 168 | 123.792 | 38.882 | 5.585 | 1.00 | 31.09 | A | C |
| ATOM | 186 | CE2 | PHE | 168 | 125.724 | 39.109 | 7.000 | 1.00 | 31.14 | A | C |
| ATOM | 187 | CZ | PHE | 168 | 125.173 | 38.906 | 5.738 | 1.00 | 33.63 | A | C |
| ATOM | 188 | C | PHE | 168 | 122.222 | 41.796 | 8.227 | 1.00 | 17.51 | A | C |
| ATOM | 189 | O | PHE | 168 | 123.139 | 42.475 | 7.750 | 1.00 | 13.95 | A | O |
| ATOM | 190 | N | LEU | 169 | 121.007 | 41.719 | 7.680 | 1.00 | 16.88 | A | N |
| ATOM | 191 | CA | LEU | 169 | 120.677 | 42.467 | 6.471 | 1.00 | 19.47 | A | C |
| ATOM | 192 | CB | LEU | 169 | 119.262 | 42.140 | 6.000 | 1.00 | 14.12 | A | C |
| ATOM | 193 | CG | LEU | 169 | 119.041 | 40.860 | 5.213 | 1.00 | 13.28 | A | C |
| ATOM | 194 | CD1 | LEU | 169 | 117.662 | 40.952 | 4.603 | 1.00 | 9.74 | A | C |
| ATOM | 195 | CD2 | LEU | 169 | 120.100 | 40.694 | 4.127 | 1.00 | 10.14 | A | C |
| ATOM | 196 | C | LEU | 169 | 120.777 | 43.966 | 6.731 | 1.00 | 21.77 | A | C |
| ATOM | 197 | O | LEU | 169 | 121.409 | 44.694 | 5.968 | 1.00 | 23.20 | A | O |
| ATOM | 198 | N | ASN | 170 | 120.150 | 44.419 | 7.815 | 1.00 | 20.45 | A | N |
| ATOM | 199 | CA | ASN | 170 | 120.159 | 45.832 | 8.175 | 1.00 | 17.58 | A | C |
| ATOM | 200 | CB | ASN | 170 | 119.534 | 46.018 | 9.562 | 1.00 | 31.53 | A | C |
| ATOM | 201 | CG | ASN | 170 | 119.017 | 47.426 | 9.791 | 1.00 | 34.95 | A | C |
| ATOM | 202 | OD1 | ASN | 170 | 119.740 | 48.282 | 10.284 | 1.00 | 30.48 | A | O |
| ATOM | 203 | ND2 | ASN | 170 | 117.762 | 47.671 | 9.421 | 1.00 | 32.86 | A | N |
| ATOM | 204 | C | ASN | 170 | 121.587 | 46.341 | 8.151 | 1.00 | 17.59 | A | C |
| ATOM | 205 | O | ASN | 170 | 121.941 | 47.174 | 7.321 | 1.00 | 17.80 | A | O |
| ATOM | 206 | N | ASP | 171 | 122.412 | 45.812 | 9.040 | 1.00 | 11.82 | A | N |
| ATOM | 207 | CA | ASP | 171 | 123.816 | 46.218 | 9.120 | 1.00 | 13.94 | A | C |
| ATOM | 208 | CB | ASP | 171 | 124.588 | 45.282 | 10.048 | 1.00 | 56.27 | A | C |
| ATOM | 209 | CG | ASP | 171 | 124.405 | 45.627 | 11.508 | 1.00 | 63.92 | A | C |
| ATOM | 210 | OD1 | ASP | 171 | 123.248 | 45.689 | 11.971 | 1.00 | 66.14 | A | O |
| ATOM | 211 | OD2 | ASP | 171 | 125.427 | 45.834 | 12.196 | 1.00 | 65.78 | A | O |
| ATOM | 212 | C | ASP | 171 | 124.509 | 46.244 | 7.760 | 1.00 | 15.43 | A | C |
| ATOM | 213 | O | ASP | 171 | 125.223 | 47.194 | 7.435 | 1.00 | 14.15 | A | O |
| ATOM | 214 | N | LEU | 172 | 124.289 | 45.200 | 6.966 | 1.00 | 15.45 | A | N |
| ATOM | 215 | CA | LEU | 172 | 124.910 | 45.099 | 5.650 | 1.00 | 16.13 | A | C |
| ATOM | 216 | CB | LEU | 172 | 124.633 | 43.717 | 5.047 | 1.00 | 10.67 | A | C |
| ATOM | 217 | CG | LEU | 172 | 125.667 | 43.058 | 4.123 | 1.00 | 10.16 | A | C |
| ATOM | 218 | CD1 | LEU | 172 | 124.905 | 42.379 | 2.979 | 1.00 | 7.76 | A | C |
| ATOM | 219 | CD2 | LEU | 172 | 126.672 | 44.070 | 3.594 | 1.00 | 8.33 | A | C |

# Fig. 19: A-4

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 220 | C | LEU | 172 | 124.401 | 46.178 | 4.699 | 1.00 | 16.47 | A | C |
| ATOM | 221 | O | LEU | 172 | 125.182 | 46.951 | 4.156 | 1.00 | 16.46 | A | O |
| ATOM | 222 | N | LEU | 173 | 123.088 | 46.226 | 4.509 | 1.00 | 30.03 | A | N |
| ATOM | 223 | CA | LEU | 173 | 122.475 | 47.193 | 3.609 | 1.00 | 32.78 | A | C |
| ATOM | 224 | CB | LEU | 173 | 120.967 | 46.932 | 3.474 | 1.00 | 23.11 | A | C |
| ATOM | 225 | CG | LEU | 173 | 120.357 | 45.803 | 2.627 | 1.00 | 24.46 | A | C |
| ATOM | 226 | CD1 | LEU | 173 | 121.069 | 45.702 | 1.292 | 1.00 | 27.98 | A | C |
| ATOM | 227 | CD2 | LEU | 173 | 120.456 | 44.501 | 3.353 | 1.00 | 25.01 | A | C |
| ATOM | 228 | C | LEU | 173 | 122.675 | 48.663 | 3.984 | 1.00 | 34.21 | A | C |
| ATOM | 229 | O | LEU | 173 | 122.937 | 49.495 | 3.105 | 1.00 | 30.93 | A | O |
| ATOM | 230 | N | LYS | 174 | 122.558 | 48.989 | 5.271 | 1.00 | 33.34 | A | N |
| ATOM | 231 | CA | LYS | 174 | 122.684 | 50.379 | 5.693 | 1.00 | 33.56 | A | C |
| ATOM | 232 | CB | LYS | 174 | 122.428 | 50.508 | 7.193 | 1.00 | 32.34 | A | C |
| ATOM | 233 | CG | LYS | 174 | 123.590 | 50.195 | 8.102 | 1.00 | 32.67 | A | C |
| ATOM | 234 | CD | LYS | 174 | 123.170 | 50.471 | 9.551 | 1.00 | 31.92 | A | C |
| ATOM | 235 | CE | LYS | 174 | 124.365 | 50.601 | 10.504 | 1.00 | 27.17 | A | C |
| ATOM | 236 | NZ | LYS | 174 | 125.178 | 49.351 | 10.664 | 1.00 | 23.64 | A | N |
| ATOM | 237 | C | LYS | 174 | 124.004 | 51.046 | 5.317 | 1.00 | 31.92 | A | C |
| ATOM | 238 | O | LYS | 174 | 124.060 | 52.256 | 5.142 | 1.00 | 32.79 | A | O |
| ATOM | 239 | N | ARG | 175 | 125.059 | 50.255 | 5.176 | 1.00 | 34.34 | A | N |
| ATOM | 240 | CA | ARG | 175 | 126.385 | 50.759 | 4.797 | 1.00 | 36.57 | A | C |
| ATOM | 241 | CB | ARG | 175 | 127.468 | 49.712 | 5.125 | 1.00 | 50.56 | A | C |
| ATOM | 242 | CG | ARG | 175 | 127.708 | 49.400 | 6.606 | 1.00 | 57.49 | A | C |
| ATOM | 243 | CD | ARG | 175 | 128.550 | 48.120 | 6.760 | 1.00 | 61.77 | A | C |
| ATOM | 244 | NE | ARG | 175 | 129.398 | 48.107 | 7.957 | 1.00 | 66.67 | A | N |
| ATOM | 245 | CZ | ARG | 175 | 128.954 | 48.049 | 9.211 | 1.00 | 70.25 | A | C |
| ATOM | 246 | NH1 | ARG | 175 | 127.653 | 47.997 | 9.461 | 1.00 | 70.45 | A | N |
| ATOM | 247 | NH2 | ARG | 175 | 129.819 | 48.039 | 10.219 | 1.00 | 71.15 | A | N |
| ATOM | 248 | C | ARG | 175 | 126.461 | 51.051 | 3.288 | 1.00 | 34.10 | A | C |
| ATOM | 249 | O | ARG | 175 | 127.487 | 51.522 | 2.796 | 1.00 | 33.94 | A | O |
| ATOM | 250 | N | MET | 176 | 125.384 | 50.766 | 2.557 | 1.00 | 18.81 | A | N |
| ATOM | 251 | CA | MET | 176 | 125.371 | 50.959 | 1.104 | 1.00 | 15.29 | A | C |
| ATOM | 252 | CB | MET | 176 | 124.758 | 49.728 | 0.431 | 1.00 | 45.67 | A | C |
| ATOM | 253 | CG | MET | 176 | 125.646 | 48.505 | 0.474 | 1.00 | 42.57 | A | C |
| ATOM | 254 | SD | MET | 176 | 124.887 | 47.063 | -0.292 | 1.00 | 46.71 | A | S |
| ATOM | 255 | CE | MET | 176 | 124.633 | 46.046 | 1.139 | 1.00 | 40.22 | A | C |
| ATOM | 256 | C | MET | 176 | 124.679 | 52.199 | 0.546 | 1.00 | 18.80 | A | C |
| ATOM | 257 | O | MET | 176 | 123.797 | 52.768 | 1.176 | 1.00 | 18.87 | A | O |
| ATOM | 258 | N | ASP | 177 | 125.098 | 52.605 | -0.652 | 1.00 | 31.75 | A | N |
| ATOM | 259 | CA | ASP | 177 | 124.504 | 53.744 | -1.344 | 1.00 | 34.24 | A | C |
| ATOM | 260 | CB | ASP | 177 | 125.584 | 54.671 | -1.903 | 1.00 | 129.70 | A | C |
| ATOM | 261 | CG | ASP | 177 | 126.196 | 55.556 | -0.838 | 1.00 | 132.65 | A | C |
| ATOM | 262 | OD1 | ASP | 177 | 127.004 | 56.437 | -1.194 | 1.00 | 132.32 | A | O |
| ATOM | 263 | OD2 | ASP | 177 | 125.869 | 55.372 | 0.354 | 1.00 | 134.30 | A | O |
| ATOM | 264 | C | ASP | 177 | 123.638 | 53.207 | -2.480 | 1.00 | 34.16 | A | C |
| ATOM | 265 | O | ASP | 177 | 124.085 | 53.107 | -3.617 | 1.00 | 33.88 | A | O |
| ATOM | 266 | N | ILE | 178 | 122.402 | 52.848 | -2.153 | 1.00 | 22.62 | A | N |
| ATOM | 267 | CA | ILE | 178 | 121.464 | 52.307 | -3.122 | 1.00 | 22.76 | A | C |
| ATOM | 268 | CB | ILE | 178 | 120.326 | 51.524 | -2.407 | 1.00 | 26.30 | A | C |
| ATOM | 269 | CG2 | ILE | 178 | 119.208 | 51.207 | -3.390 | 1.00 | 24.58 | A | C |
| ATOM | 270 | CG1 | ILE | 178 | 120.866 | 50.222 | -1.803 | 1.00 | 27.36 | A | C |
| ATOM | 271 | CD1 | ILE | 178 | 121.188 | 50.292 | -0.325 | 1.00 | 29.20 | A | C |
| ATOM | 272 | C | ILE | 178 | 120.848 | 53.398 | -4.009 | 1.00 | 21.90 | A | C |
| ATOM | 273 | O | ILE | 178 | 120.532 | 54.501 | -3.539 | 1.00 | 23.89 | A | O |
| ATOM | 274 | N | GLY | 179 | 120.669 | 53.077 | -5.292 | 1.00 | 18.17 | A | N |
| ATOM | 275 | CA | GLY | 179 | 120.091 | 54.029 | -6.226 | 1.00 | 17.89 | A | C |
| ATOM | 276 | C | GLY | 179 | 120.123 | 53.536 | -7.658 | 1.00 | 18.65 | A | C |
| ATOM | 277 | O | GLY | 179 | 121.019 | 52.786 | -8.023 | 1.00 | 16.80 | A | O |
| ATOM | 278 | N | PRO | 180 | 119.150 | 53.937 | -8.498 | 1.00 | 18.34 | A | N |
| ATOM | 279 | CD | PRO | 180 | 117.980 | 54.770 | -8.159 | 1.00 | 16.60 | A | C |
| ATOM | 280 | CA | PRO | 180 | 119.094 | 53.512 | -9.901 | 1.00 | 19.40 | A | C |
| ATOM | 281 | CB | PRO | 180 | 118.044 | 54.442 | -10.498 | 1.00 | 15.44 | A | C |
| ATOM | 282 | CG | PRO | 180 | 117.074 | 54.573 | -9.365 | 1.00 | 17.83 | A | C |
| ATOM | 283 | C | PRO | 180 | 120.432 | 53.622 | -10.597 | 1.00 | 21.18 | A | C |
| ATOM | 284 | O | PRO | 180 | 120.706 | 52.877 | -11.529 | 1.00 | 21.82 | A | O |
| ATOM | 285 | N | LYS | 181 | 121.262 | 54.553 | -10.139 | 1.00 | 25.85 | A | N |
| ATOM | 286 | CA | LYS | 181 | 122.581 | 54.751 | -10.732 | 1.00 | 26.27 | A | C |
| ATOM | 287 | CB | LYS | 181 | 122.737 | 56.187 | -11.253 | 1.00 | 26.21 | A | C |
| ATOM | 288 | CG | LYS | 181 | 121.801 | 56.557 | -12.403 | 1.00 | 26.81 | A | C |
| ATOM | 289 | CD | LYS | 181 | 122.014 | 55.683 | -13.627 | 1.00 | 25.67 | A | C |
| ATOM | 290 | CE | LYS | 181 | 121.014 | 56.031 | -14.719 | 1.00 | 28.19 | A | C |
| ATOM | 291 | NZ | LYS | 181 | 121.097 | 55.146 | -15.923 | 1.00 | 27.76 | A | N |
| ATOM | 292 | C | LYS | 181 | 123.684 | 54.451 | -9.729 | 1.00 | 25.62 | A | C |

Fig. 19: A-5

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 293 | O | LYS | 181 | 124.854 | 54.742 | -9.975 | 1.00 | 23.94 | A | O |
| ATOM | 294 | N | GLN | 182 | 123.300 | 53.870 | -8.599 | 1.00 | 34.95 | A | N |
| ATOM | 295 | CA | GLN | 182 | 124.246 | 53.513 | -7.548 | 1.00 | 33.61 | A | C |
| ATOM | 296 | CB | GLN | 182 | 123.797 | 54.096 | -6.207 | 1.00 | 89.66 | A | C |
| ATOM | 297 | CG | GLN | 182 | 123.331 | 55.528 | -6.251 | 1.00 | 90.94 | A | C |
| ATOM | 298 | CD | GLN | 182 | 124.443 | 56.478 | -6.597 | 1.00 | 92.56 | A | C |
| ATOM | 299 | OE1 | GLN | 182 | 125.007 | 56.418 | -7.686 | 1.00 | 93.40 | A | O |
| ATOM | 300 | NE2 | GLN | 182 | 124.772 | 57.364 | -5.667 | 1.00 | 93.92 | A | N |
| ATOM | 301 | C | GLN | 182 | 124.258 | 51.991 | -7.439 | 1.00 | 32.52 | A | C |
| ATOM | 302 | O | GLN | 182 | 124.398 | 51.278 | -8.429 | 1.00 | 36.85 | A | O |
| ATOM | 303 | N | THR | 183 | 124.096 | 51.507 | -6.216 | 1.00 | 26.87 | A | N |
| ATOM | 304 | CA | THR | 183 | 124.052 | 50.083 | -5.953 | 1.00 | 23.79 | A | C |
| ATOM | 305 | CB | THR | 183 | 124.642 | 49.767 | -4.584 | 1.00 | 30.55 | A | C |
| ATOM | 306 | OG1 | THR | 183 | 125.983 | 50.262 | -4.526 | 1.00 | 27.00 | A | O |
| ATOM | 307 | CG2 | THR | 183 | 124.629 | 48.274 | -4.331 | 1.00 | 28.23 | A | C |
| ATOM | 308 | C | THR | 183 | 122.590 | 49.687 | -5.944 | 1.00 | 23.45 | A | C |
| ATOM | 309 | O | THR | 183 | 121.752 | 50.380 | -5.368 | 1.00 | 21.98 | A | O |
| ATOM | 310 | N | GLN | 184 | 122.269 | 48.592 | -6.608 | 1.00 | 25.73 | A | N |
| ATOM | 311 | CA | GLN | 184 | 120.897 | 48.127 | -6.612 | 1.00 | 21.38 | A | C |
| ATOM | 312 | CB | GLN | 184 | 120.399 | 47.898 | -8.042 | 1.00 | 35.06 | A | C |
| ATOM | 313 | CG | GLN | 184 | 120.016 | 49.181 | -8.770 | 1.00 | 34.81 | A | C |
| ATOM | 314 | CD | GLN | 184 | 118.982 | 48.942 | -9.856 | 1.00 | 34.28 | A | C |
| ATOM | 315 | OE1 | GLN | 184 | 119.215 | 48.164 | -10.781 | 1.00 | 29.98 | A | O |
| ATOM | 316 | NE2 | GLN | 184 | 117.834 | 49.604 | -9.748 | 1.00 | 32.58 | A | N |
| ATOM | 317 | C | GLN | 184 | 120.862 | 46.839 | -5.800 | 1.00 | 21.76 | A | C |
| ATOM | 318 | O | GLN | 184 | 121.832 | 46.087 | -5.780 | 1.00 | 19.15 | A | O |
| ATOM | 319 | N | VAL | 185 | 119.753 | 46.599 | -5.112 | 1.00 | 33.23 | A | N |
| ATOM | 320 | CA | VAL | 185 | 119.634 | 45.408 | -4.298 | 1.00 | 31.60 | A | C |
| ATOM | 321 | CB | VAL | 185 | 119.868 | 45.742 | -2.810 | 1.00 | 20.42 | A | C |
| ATOM | 322 | CG1 | VAL | 185 | 119.572 | 44.535 | -1.938 | 1.00 | 20.41 | A | C |
| ATOM | 323 | CG2 | VAL | 185 | 121.294 | 46.148 | -2.614 | 1.00 | 6.28 | A | C |
| ATOM | 324 | C | VAL | 185 | 118.297 | 44.701 | -4.445 | 1.00 | 32.19 | A | C |
| ATOM | 325 | O | VAL | 185 | 117.237 | 45.322 | -4.469 | 1.00 | 29.34 | A | O |
| ATOM | 326 | N | GLY | 186 | 118.369 | 43.382 | -4.554 | 1.00 | 17.76 | A | N |
| ATOM | 327 | CA | GLY | 186 | 117.177 | 42.573 | -4.672 | 1.00 | 19.39 | A | C |
| ATOM | 328 | C | GLY | 186 | 117.355 | 41.424 | -3.711 | 1.00 | 17.37 | A | C |
| ATOM | 329 | O | GLY | 186 | 118.470 | 40.929 | -3.543 | 1.00 | 22.73 | A | O |
| ATOM | 330 | N | ILE | 187 | 116.278 | 40.995 | -3.073 | 1.00 | 15.41 | A | N |
| ATOM | 331 | CA | ILE | 187 | 116.395 | 39.906 | -2.133 | 1.00 | 14.00 | A | C |
| ATOM | 332 | CB | ILE | 187 | 116.117 | 40.403 | -0.675 | 1.00 | 10.12 | A | C |
| ATOM | 333 | CG2 | ILE | 187 | 116.053 | 39.225 | 0.299 | 1.00 | 7.45 | A | C |
| ATOM | 334 | CG1 | ILE | 187 | 117.232 | 41.364 | -0.253 | 1.00 | 10.64 | A | C |
| ATOM | 335 | CD1 | ILE | 187 | 117.156 | 41.817 | 1.176 | 1.00 | 11.69 | A | C |
| ATOM | 336 | C | ILE | 187 | 115.496 | 38.731 | -2.485 | 1.00 | 13.29 | A | C |
| ATOM | 337 | O | ILE | 187 | 114.301 | 38.896 | -2.768 | 1.00 | 12.19 | A | O |
| ATOM | 338 | N | VAL | 188 | 116.097 | 37.546 | -2.473 | 1.00 | 16.67 | A | N |
| ATOM | 339 | CA | VAL | 188 | 115.403 | 36.303 | -2.769 | 1.00 | 16.34 | A | C |
| ATOM | 340 | CB | VAL | 188 | 116.082 | 35.567 | -3.951 | 1.00 | 11.96 | A | C |
| ATOM | 341 | CG1 | VAL | 188 | 115.642 | 34.122 | -3.993 | 1.00 | 7.23 | A | C |
| ATOM | 342 | CG2 | VAL | 188 | 115.742 | 36.251 | -5.248 | 1.00 | 12.38 | A | C |
| ATOM | 343 | C | VAL | 188 | 115.464 | 35.404 | -1.536 | 1.00 | 14.88 | A | C |
| ATOM | 344 | O | VAL | 188 | 116.509 | 35.286 | -0.895 | 1.00 | 14.29 | A | O |
| ATOM | 345 | N | GLN | 189 | 114.348 | 34.774 | -1.194 | 1.00 | 30.23 | A | N |
| ATOM | 346 | CA | GLN | 189 | 114.335 | 33.873 | -0.049 | 1.00 | 29.91 | A | C |
| ATOM | 347 | CB | GLN | 189 | 113.374 | 34.363 | 1.039 | 1.00 | 26.02 | A | C |
| ATOM | 348 | CG | GLN | 189 | 113.277 | 33.399 | 2.210 | 1.00 | 23.53 | A | C |
| ATOM | 349 | CD | GLN | 189 | 112.257 | 33.807 | 3.267 | 1.00 | 24.24 | A | C |
| ATOM | 350 | OE1 | GLN | 189 | 111.891 | 32.998 | 4.125 | 1.00 | 25.46 | A | O |
| ATOM | 351 | NE2 | GLN | 189 | 111.800 | 35.058 | 3.219 | 1.00 | 25.28 | A | N |
| ATOM | 352 | C | GLN | 189 | 113.911 | 32.490 | -0.520 | 1.00 | 26.90 | A | C |
| ATOM | 353 | O | GLN | 189 | 113.056 | 32.366 | -1.401 | 1.00 | 25.26 | A | O |
| ATOM | 354 | N | TYR | 190 | 114.516 | 31.455 | 0.063 | 1.00 | 12.87 | A | N |
| ATOM | 355 | CA | TYR | 190 | 114.196 | 30.084 | -0.310 | 1.00 | 16.39 | A | C |
| ATOM | 356 | CB | TYR | 190 | 115.267 | 29.539 | -1.257 | 1.00 | 17.86 | A | C |
| ATOM | 357 | CG | TYR | 190 | 116.599 | 29.241 | -0.590 | 1.00 | 13.63 | A | C |
| ATOM | 358 | CD1 | TYR | 190 | 116.887 | 27.963 | -0.092 | 1.00 | 13.63 | A | C |
| ATOM | 359 | CE1 | TYR | 190 | 118.104 | 27.687 | 0.517 | 1.00 | 13.63 | A | C |
| ATOM | 360 | CD2 | TYR | 190 | 117.569 | 30.233 | -0.453 | 1.00 | 13.63 | A | C |
| ATOM | 361 | CE2 | TYR | 190 | 118.787 | 29.968 | 0.159 | 1.00 | 13.63 | A | C |
| ATOM | 362 | CZ | TYR | 190 | 119.053 | 28.698 | 0.640 | 1.00 | 13.63 | A | C |
| ATOM | 363 | OH | TYR | 190 | 120.278 | 28.442 | 1.228 | 1.00 | 13.63 | A | O |
| ATOM | 364 | C | TYR | 190 | 114.035 | 29.135 | 0.878 | 1.00 | 18.24 | A | C |
| ATOM | 365 | O | TYR | 190 | 114.456 | 29.424 | 2.003 | 1.00 | 18.32 | A | O |

# Fig. 19: A-6

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 366 | N | GLY | 191 | 113.417 | 27.994 | 0.588 | 1.00 | 15.40 | A | N |
| ATOM | 367 | CA | GLY | 191 | 113.171 | 26.954 | 1.572 | 1.00 | 13.15 | A | C |
| ATOM | 368 | C | GLY | 191 | 112.683 | 25.776 | 0.764 | 1.00 | 14.59 | A | C |
| ATOM | 369 | O | GLY | 191 | 113.482 | 25.084 | 0.139 | 1.00 | 17.97 | A | O |
| ATOM | 370 | N | GLU | 192 | 111.371 | 25.552 | 0.769 | 1.00 | 27.03 | A | N |
| ATOM | 371 | CA | GLU | 192 | 110.764 | 24.475 | -0.020 | 1.00 | 29.04 | A | C |
| ATOM | 372 | CB | GLU | 192 | 109.400 | 24.089 | 0.537 | 1.00 | 28.96 | A | C |
| ATOM | 373 | CG | GLU | 192 | 109.412 | 23.507 | 1.929 | 1.00 | 29.34 | A | C |
| ATOM | 374 | CD | GLU | 192 | 108.020 | 23.089 | 2.390 | 1.00 | 29.53 | A | C |
| ATOM | 375 | OE1 | GLU | 192 | 107.890 | 22.532 | 3.505 | 1.00 | 32.42 | A | O |
| ATOM | 376 | OE2 | GLU | 192 | 107.051 | 23.322 | 1.633 | 1.00 | 27.40 | A | O |
| ATOM | 377 | C | GLU | 192 | 110.562 | 25.062 | -1.410 | 1.00 | 28.85 | A | C |
| ATOM | 378 | O | GLU | 192 | 110.692 | 24.380 | -2.422 | 1.00 | 30.22 | A | O |
| ATOM | 379 | N | ASN | 193 | 110.236 | 26.350 | -1.433 | 1.00 | 34.68 | A | N |
| ATOM | 380 | CA | ASN | 193 | 110.019 | 27.088 | -2.668 | 1.00 | 35.89 | A | C |
| ATOM | 381 | CB | ASN | 193 | 108.566 | 27.527 | -2.769 | 1.00 | 60.91 | A | C |
| ATOM | 382 | CG | ASN | 193 | 107.606 | 26.388 | -2.564 | 1.00 | 64.08 | A | C |
| ATOM | 383 | OD1 | ASN | 193 | 107.545 | 25.804 | -1.488 | 1.00 | 68.19 | A | O |
| ATOM | 384 | ND2 | ASN | 193 | 106.849 | 26.058 | -3.601 | 1.00 | 66.19 | A | N |
| ATOM | 385 | C | ASN | 193 | 110.910 | 28.315 | -2.640 | 1.00 | 34.07 | A | C |
| ATOM | 386 | O | ASN | 193 | 111.759 | 28.459 | -1.760 | 1.00 | 35.07 | A | O |
| ATOM | 387 | N | VAL | 194 | 110.712 | 29.206 | -3.598 | 1.00 | 31.94 | A | N |
| ATOM | 388 | CA | VAL | 194 | 111.511 | 30.423 | -3.660 | 1.00 | 34.28 | A | C |
| ATOM | 389 | CB | VAL | 194 | 112.524 | 30.365 | -4.803 | 1.00 | 32.89 | A | C |
| ATOM | 390 | CG1 | VAL | 194 | 113.514 | 31.495 | -4.671 | 1.00 | 33.92 | A | C |
| ATOM | 391 | CG2 | VAL | 194 | 113.227 | 29.036 | -4.799 | 1.00 | 30.16 | A | C |
| ATOM | 392 | C | VAL | 194 | 110.601 | 31.608 | -3.914 | 1.00 | 32.05 | A | C |
| ATOM | 393 | O | VAL | 194 | 109.651 | 31.507 | -4.688 | 1.00 | 30.17 | A | O |
| ATOM | 394 | N | THR | 195 | 110.877 | 32.730 | -3.261 | 1.00 | 26.46 | A | N |
| ATOM | 395 | CA | THR | 195 | 110.058 | 33.915 | -3.474 | 1.00 | 27.64 | A | C |
| ATOM | 396 | CB | THR | 195 | 109.050 | 34.135 | -2.307 | 1.00 | 36.45 | A | C |
| ATOM | 397 | OG1 | THR | 195 | 109.728 | 34.654 | -1.163 | 1.00 | 40.46 | A | O |
| ATOM | 398 | CG2 | THR | 195 | 108.396 | 32.820 | -1.918 | 1.00 | 38.08 | A | C |
| ATOM | 399 | C | THR | 195 | 110.927 | 35.161 | -3.656 | 1.00 | 28.48 | A | C |
| ATOM | 400 | O | THR | 195 | 111.977 | 35.309 | -3.032 | 1.00 | 31.07 | A | O |
| ATOM | 401 | N | HIS | 196 | 110.492 | 36.040 | -4.545 | 1.00 | 36.83 | A | N |
| ATOM | 402 | CA | HIS | 196 | 111.196 | 37.281 | -4.819 | 1.00 | 36.93 | A | C |
| ATOM | 403 | CB | HIS | 196 | 110.843 | 37.772 | -6.225 | 1.00 | 33.18 | A | C |
| ATOM | 404 | CG | HIS | 196 | 111.434 | 36.951 | -7.326 | 1.00 | 29.68 | A | C |
| ATOM | 405 | CD2 | HIS | 196 | 110.933 | 35.910 | -8.032 | 1.00 | 30.31 | A | C |
| ATOM | 406 | ND1 | HIS | 196 | 112.707 | 37.169 | -7.813 | 1.00 | 28.33 | A | N |
| ATOM | 407 | CE1 | HIS | 196 | 112.965 | 36.296 | -8.772 | 1.00 | 25.05 | A | C |
| ATOM | 408 | NE2 | HIS | 196 | 111.905 | 35.521 | -8.924 | 1.00 | 23.26 | A | N |
| ATOM | 409 | C | HIS | 196 | 110.730 | 38.315 | -3.802 | 1.00 | 36.79 | A | C |
| ATOM | 410 | O | HIS | 196 | 109.687 | 38.933 | -3.997 | 1.00 | 35.45 | A | O |
| ATOM | 411 | N | GLU | 197 | 111.480 | 38.508 | -2.721 | 1.00 | 21.51 | A | N |
| ATOM | 412 | CA | GLU | 197 | 111.069 | 39.488 | -1.732 | 1.00 | 18.84 | A | C |
| ATOM | 413 | CB | GLU | 197 | 112.091 | 39.588 | -0.604 | 1.00 | 43.52 | A | C |
| ATOM | 414 | CG | GLU | 197 | 112.094 | 38.384 | 0.339 | 1.00 | 43.86 | A | C |
| ATOM | 415 | CD | GLU | 197 | 110.717 | 38.043 | 0.882 | 1.00 | 42.93 | A | C |
| ATOM | 416 | OE1 | GLU | 197 | 109.909 | 38.967 | 1.100 | 1.00 | 41.51 | A | O |
| ATOM | 417 | OE2 | GLU | 197 | 110.444 | 36.847 | 1.111 | 1.00 | 44.59 | A | O |
| ATOM | 418 | C | GLU | 197 | 110.882 | 40.832 | -2.442 | 1.00 | 16.31 | A | C |
| ATOM | 419 | O | GLU | 197 | 109.802 | 41.419 | -2.403 | 1.00 | 21.51 | A | O |
| ATOM | 420 | N | PHE | 198 | 111.921 | 41.325 | -3.098 | 1.00 | 11.53 | A | N |
| ATOM | 421 | CA | PHE | 198 | 111.786 | 42.562 | -3.845 | 1.00 | 13.33 | A | C |
| ATOM | 422 | CB | PHE | 198 | 111.803 | 43.785 | -2.901 | 1.00 | 15.90 | A | C |
| ATOM | 423 | CG | PHE | 198 | 113.092 | 44.003 | -2.153 | 1.00 | 14.15 | A | C |
| ATOM | 424 | CD1 | PHE | 198 | 114.262 | 44.390 | -2.823 | 1.00 | 20.29 | A | C |
| ATOM | 425 | CD2 | PHE | 198 | 113.115 | 43.912 | -0.756 | 1.00 | 10.34 | A | C |
| ATOM | 426 | CE1 | PHE | 198 | 115.427 | 44.685 | -2.113 | 1.00 | 16.32 | A | C |
| ATOM | 427 | CE2 | PHE | 198 | 114.274 | 44.208 | -0.039 | 1.00 | 14.80 | A | C |
| ATOM | 428 | CZ | PHE | 198 | 115.431 | 44.594 | -0.719 | 1.00 | 18.60 | A | C |
| ATOM | 429 | C | PHE | 198 | 112.829 | 42.652 | -4.956 | 1.00 | 16.01 | A | C |
| ATOM | 430 | O | PHE | 198 | 113.974 | 42.239 | -4.771 | 1.00 | 17.30 | A | O |
| ATOM | 431 | N | ASN | 199 | 112.418 | 43.152 | -6.123 | 1.00 | 19.42 | A | N |
| ATOM | 432 | CA | ASN | 199 | 113.321 | 43.265 | -7.276 | 1.00 | 19.71 | A | C |
| ATOM | 433 | CB | ASN | 199 | 112.540 | 43.562 | -8.548 | 1.00 | 30.06 | A | C |
| ATOM | 434 | CG | ASN | 199 | 111.465 | 42.548 | -8.824 | 1.00 | 31.32 | A | C |
| ATOM | 435 | OD1 | ASN | 199 | 111.726 | 41.350 | -8.934 | 1.00 | 32.85 | A | O |
| ATOM | 436 | ND2 | ASN | 199 | 110.236 | 43.029 | -8.948 | 1.00 | 30.20 | A | N |
| ATOM | 437 | C | ASN | 199 | 114.458 | 44.288 | -7.173 | 1.00 | 22.17 | A | C |
| ATOM | 438 | O | ASN | 199 | 114.430 | 45.215 | -6.351 | 1.00 | 19.98 | A | O |

Fig. 19: A-7

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 439 | N | LEU | 200 | 115.445 | 44.107 | -8.044 | 1.00 | 18.99 | A | N |
| ATOM | 440 | CA | LEU | 200 | 116.619 | 44.958 | -8.078 | 1.00 | 20.95 | A | C |
| ATOM | 441 | CB | LEU | 200 | 117.556 | 44.524 | -9.212 | 1.00 | 24.87 | A | C |
| ATOM | 442 | CG | LEU | 200 | 118.631 | 43.490 | -8.869 | 1.00 | 22.72 | A | C |
| ATOM | 443 | CD1 | LEU | 200 | 119.348 | 43.048 | -10.130 | 1.00 | 27.84 | A | C |
| ATOM | 444 | CD2 | LEU | 200 | 119.617 | 44.089 | -7.869 | 1.00 | 23.89 | A | C |
| ATOM | 445 | C | LEU | 200 | 116.282 | 46.415 | -8.246 | 1.00 | 21.35 | A | C |
| ATOM | 446 | O | LEU | 200 | 116.960 | 47.274 | -7.688 | 1.00 | 22.37 | A | O |
| ATOM | 447 | N | ASN | 201 | 115.231 | 46.691 | -9.011 | 1.00 | 18.94 | A | N |
| ATOM | 448 | CA | ASN | 201 | 114.816 | 48.061 | -9.284 | 1.00 | 20.79 | A | C |
| ATOM | 449 | CB | ASN | 201 | 114.546 | 48.208 | -10.773 | 1.00 | 21.69 | A | C |
| ATOM | 450 | CG | ASN | 201 | 113.401 | 47.336 | -11.236 | 1.00 | 23.97 | A | C |
| ATOM | 451 | OD1 | ASN | 201 | 113.119 | 47.246 | -12.424 | 1.00 | 24.11 | A | O |
| ATOM | 452 | ND2 | ASN | 201 | 112.727 | 46.684 | -10.292 | 1.00 | 21.81 | A | N |
| ATOM | 453 | C | ASN | 201 | 113.572 | 48.510 | -8.509 | 1.00 | 20.84 | A | C |
| ATOM | 454 | O | ASN | 201 | 112.969 | 49.522 | -8.851 | 1.00 | 16.74 | A | O |
| ATOM | 455 | N | LYS | 202 | 113.182 | 47.770 | -7.477 | 1.00 | 23.30 | A | N |
| ATOM | 456 | CA | LYS | 202 | 111.998 | 48.137 | -6.710 | 1.00 | 23.42 | A | C |
| ATOM | 457 | CB | LYS | 202 | 111.621 | 47.022 | -5.741 | 1.00 | 34.18 | A | C |
| ATOM | 458 | CG | LYS | 202 | 110.337 | 47.265 | -4.944 | 1.00 | 35.72 | A | C |
| ATOM | 459 | CD | LYS | 202 | 109.099 | 47.092 | -5.803 | 1.00 | 37.63 | A | C |
| ATOM | 460 | CE | LYS | 202 | 109.162 | 45.813 | -6.678 | 1.00 | 43.38 | A | C |
| ATOM | 461 | NZ | LYS | 202 | 109.316 | 44.491 | -5.962 | 1.00 | 42.40 | A | N |
| ATOM | 462 | C | LYS | 202 | 112.188 | 49.428 | -5.930 | 1.00 | 22.29 | A | C |
| ATOM | 463 | O | LYS | 202 | 111.338 | 50.313 | -5.984 | 1.00 | 19.57 | A | O |
| ATOM | 464 | N | TYR | 203 | 113.292 | 49.538 | -5.203 | 1.00 | 24.72 | A | N |
| ATOM | 465 | CA | TYR | 203 | 113.538 | 50.731 | -4.407 | 1.00 | 24.40 | A | C |
| ATOM | 466 | CB | TYR | 203 | 113.769 | 50.348 | -2.942 | 1.00 | 32.57 | A | C |
| ATOM | 467 | CG | TYR | 203 | 112.679 | 49.461 | -2.396 | 1.00 | 31.24 | A | C |
| ATOM | 468 | CD1 | TYR | 203 | 112.869 | 48.086 | -2.282 | 1.00 | 31.85 | A | C |
| ATOM | 469 | CE1 | TYR | 203 | 111.842 | 47.251 | -1.844 | 1.00 | 28.32 | A | C |
| ATOM | 470 | CD2 | TYR | 203 | 111.427 | 49.986 | -2.050 | 1.00 | 34.13 | A | C |
| ATOM | 471 | CE2 | TYR | 203 | 110.393 | 49.161 | -1.611 | 1.00 | 36.88 | A | C |
| ATOM | 472 | CZ | TYR | 203 | 110.607 | 47.794 | -1.512 | 1.00 | 36.50 | A | C |
| ATOM | 473 | OH | TYR | 203 | 109.590 | 46.962 | -1.095 | 1.00 | 41.50 | A | O |
| ATOM | 474 | C | TYR | 203 | 114.713 | 51.541 | -4.938 | 1.00 | 25.04 | A | C |
| ATOM | 475 | O | TYR | 203 | 115.755 | 50.986 | -5.280 | 1.00 | 23.21 | A | O |
| ATOM | 476 | N | SER | 204 | 114.536 | 52.861 | -4.998 | 1.00 | 28.94 | A | N |
| ATOM | 477 | CA | SER | 204 | 115.557 | 53.764 | -5.513 | 1.00 | 30.79 | A | C |
| ATOM | 478 | CB | SER | 204 | 114.892 | 54.863 | -6.338 | 1.00 | 29.83 | A | C |
| ATOM | 479 | OG | SER | 204 | 113.945 | 55.577 | -5.558 | 1.00 | 31.66 | A | O |
| ATOM | 480 | C | SER | 204 | 116.372 | 54.402 | -4.412 | 1.00 | 33.37 | A | C |
| ATOM | 481 | O | SER | 204 | 117.247 | 55.214 | -4.680 | 1.00 | 33.88 | A | O |
| ATOM | 482 | N | SER | 205 | 116.089 | 54.027 | -3.173 | 1.00 | 27.33 | A | N |
| ATOM | 483 | CA | SER | 205 | 116.787 | 54.615 | -2.048 | 1.00 | 26.99 | A | C |
| ATOM | 484 | CB | SER | 205 | 115.874 | 55.628 | -1.378 | 1.00 | 50.70 | A | C |
| ATOM | 485 | OG | SER | 205 | 116.409 | 56.032 | -0.137 | 1.00 | 56.19 | A | O |
| ATOM | 486 | C | SER | 205 | 117.251 | 53.608 | -1.016 | 1.00 | 25.12 | A | C |
| ATOM | 487 | O | SER | 205 | 116.650 | 52.551 | -0.857 | 1.00 | 21.38 | A | O |
| ATOM | 488 | N | THR | 206 | 118.318 | 53.949 | -0.301 | 1.00 | 23.44 | A | N |
| ATOM | 489 | CA | THR | 206 | 118.854 | 53.075 | 0.735 | 1.00 | 24.79 | A | C |
| ATOM | 490 | CB | THR | 206 | 120.176 | 53.614 | 1.286 | 1.00 | 12.85 | A | C |
| ATOM | 491 | OG1 | THR | 206 | 121.137 | 53.683 | 0.227 | 1.00 | 11.66 | A | O |
| ATOM | 492 | CG2 | THR | 206 | 120.696 | 52.712 | 2.392 | 1.00 | 11.22 | A | C |
| ATOM | 493 | C | THR | 206 | 117.889 | 52.879 | 1.900 | 1.00 | 25.38 | A | C |
| ATOM | 494 | O | THR | 206 | 117.798 | 51.785 | 2.447 | 1.00 | 28.17 | A | O |
| ATOM | 495 | N | GLU | 207 | 117.173 | 53.926 | 2.299 | 1.00 | 23.18 | A | N |
| ATOM | 496 | CA | GLU | 207 | 116.238 | 53.746 | 3.394 | 1.00 | 22.34 | A | C |
| ATOM | 497 | CB | GLU | 207 | 115.800 | 55.083 | 3.986 | 1.00 | 114.79 | A | C |
| ATOM | 498 | CG | GLU | 207 | 115.317 | 56.095 | 2.992 | 1.00 | 115.51 | A | C |
| ATOM | 499 | CD | GLU | 207 | 114.757 | 57.325 | 3.675 | 1.00 | 116.92 | A | C |
| ATOM | 500 | OE1 | GLU | 207 | 115.428 | 57.857 | 4.587 | 1.00 | 116.15 | A | O |
| ATOM | 501 | OE2 | GLU | 207 | 113.648 | 57.761 | 3.302 | 1.00 | 115.82 | A | O |
| ATOM | 502 | C | GLU | 207 | 115.038 | 52.937 | 2.908 | 1.00 | 22.84 | A | C |
| ATOM | 503 | O | GLU | 207 | 114.515 | 52.094 | 3.640 | 1.00 | 22.79 | A | O |
| ATOM | 504 | N | GLU | 208 | 114.614 | 53.163 | 1.668 | 1.00 | 31.71 | A | N |
| ATOM | 505 | CA | GLU | 208 | 113.485 | 52.412 | 1.126 | 1.00 | 33.44 | A | C |
| ATOM | 506 | CB | GLU | 208 | 113.168 | 52.841 | -0.308 | 1.00 | 38.62 | A | C |
| ATOM | 507 | CG | GLU | 208 | 112.661 | 54.265 | -0.441 | 1.00 | 36.09 | A | C |
| ATOM | 508 | CD | GLU | 208 | 112.288 | 54.633 | -1.875 | 1.00 | 35.61 | A | C |
| ATOM | 509 | OE1 | GLU | 208 | 111.943 | 55.811 | -2.111 | 1.00 | 41.38 | A | O |
| ATOM | 510 | OE2 | GLU | 208 | 112.338 | 53.757 | -2.767 | 1.00 | 34.33 | A | O |
| ATOM | 511 | C | GLU | 208 | 113.808 | 50.920 | 1.148 | 1.00 | 34.14 | A | C |

# Fig. 19: A-8

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 512 | O | GLU | 208 | 112.942 | 50.093 | 1.426 | 1.00 | 35.14 | A | O |
| ATOM | 513 | N | VAL | 209 | 115.057 | 50.575 | 0.855 | 1.00 | 17.60 | A | N |
| ATOM | 514 | CA | VAL | 209 | 115.472 | 49.180 | 0.853 | 1.00 | 16.52 | A | C |
| ATOM | 515 | CB | VAL | 209 | 116.790 | 48.982 | 0.077 | 1.00 | 10.63 | A | C |
| ATOM | 516 | CG1 | VAL | 209 | 117.501 | 47.719 | 0.538 | 1.00 | 10.96 | A | C |
| ATOM | 517 | CG2 | VAL | 209 | 116.491 | 48.889 | -1.398 | 1.00 | 11.65 | A | C |
| ATOM | 518 | C | VAL | 209 | 115.656 | 48.691 | 2.276 | 1.00 | 14.54 | A | C |
| ATOM | 519 | O | VAL | 209 | 115.278 | 47.558 | 2.596 | 1.00 | 13.50 | A | O |
| ATOM | 520 | N | LEU | 210 | 116.230 | 49.548 | 3.123 | 1.00 | 19.45 | A | N |
| ATOM | 521 | CA | LEU | 210 | 116.459 | 49.205 | 4.521 | 1.00 | 19.78 | A | C |
| ATOM | 522 | CB | LEU | 210 | 117.148 | 50.354 | 5.242 | 1.00 | 21.61 | A | C |
| ATOM | 523 | CG | LEU | 210 | 118.589 | 50.100 | 5.683 | 1.00 | 21.85 | A | C |
| ATOM | 524 | CD1 | LEU | 210 | 119.093 | 51.347 | 6.358 | 1.00 | 18.40 | A | C |
| ATOM | 525 | CD2 | LEU | 210 | 118.687 | 48.916 | 6.632 | 1.00 | 15.30 | A | C |
| ATOM | 526 | C | LEU | 210 | 115.148 | 48.894 | 5.223 | 1.00 | 18.04 | A | C |
| ATOM | 527 | O | LEU | 210 | 115.078 | 48.022 | 6.093 | 1.00 | 18.81 | A | O |
| ATOM | 528 | N | VAL | 211 | 114.107 | 49.618 | 4.839 | 1.00 | 25.49 | A | N |
| ATOM | 529 | CA | VAL | 211 | 112.798 | 49.443 | 5.432 | 1.00 | 25.25 | A | C |
| ATOM | 530 | CB | VAL | 211 | 111.916 | 50.685 | 5.175 | 1.00 | 19.83 | A | C |
| ATOM | 531 | CG1 | VAL | 211 | 110.457 | 50.391 | 5.537 | 1.00 | 22.01 | A | C |
| ATOM | 532 | CG2 | VAL | 211 | 112.446 | 51.859 | 5.989 | 1.00 | 20.44 | A | C |
| ATOM | 533 | C | VAL | 211 | 112.107 | 48.214 | 4.871 | 1.00 | 24.50 | A | C |
| ATOM | 534 | O | VAL | 211 | 111.437 | 47.483 | 5.593 | 1.00 | 25.18 | A | O |
| ATOM | 535 | N | ALA | 212 | 112.262 | 47.986 | 3.577 | 1.00 | 29.23 | A | N |
| ATOM | 536 | CA | ALA | 212 | 111.624 | 46.839 | 2.964 | 1.00 | 28.21 | A | C |
| ATOM | 537 | CB | ALA | 212 | 111.725 | 46.935 | 1.439 | 1.00 | 1.87 | A | C |
| ATOM | 538 | C | ALA | 212 | 112.275 | 45.559 | 3.465 | 1.00 | 26.02 | A | C |
| ATOM | 539 | O | ALA | 212 | 111.603 | 44.543 | 3.657 | 1.00 | 25.96 | A | O |
| ATOM | 540 | N | ALA | 213 | 113.587 | 45.618 | 3.680 | 1.00 | 33.07 | A | N |
| ATOM | 541 | CA | ALA | 213 | 114.339 | 44.464 | 4.147 | 1.00 | 34.24 | A | C |
| ATOM | 542 | CB | ALA | 213 | 115.803 | 44.787 | 4.176 | 1.00 | 20.72 | A | C |
| ATOM | 543 | C | ALA | 213 | 113.875 | 44.011 | 5.522 | 1.00 | 33.04 | A | C |
| ATOM | 544 | O | ALA | 213 | 113.659 | 42.824 | 5.746 | 1.00 | 30.67 | A | O |
| ATOM | 545 | N | ASN | 214 | 113.723 | 44.952 | 6.446 | 1.00 | 10.19 | A | N |
| ATOM | 546 | CA | ASN | 214 | 113.268 | 44.608 | 7.788 | 1.00 | 14.06 | A | C |
| ATOM | 547 | CB | ASN | 214 | 113.357 | 45.817 | 8.713 | 1.00 | 18.34 | A | C |
| ATOM | 548 | CG | ASN | 214 | 114.763 | 46.094 | 9.158 | 1.00 | 20.07 | A | C |
| ATOM | 549 | OD1 | ASN | 214 | 115.597 | 46.563 | 8.377 | 1.00 | 22.00 | A | O |
| ATOM | 550 | ND2 | ASN | 214 | 115.045 | 45.794 | 10.425 | 1.00 | 20.49 | A | N |
| ATOM | 551 | C | ASN | 214 | 111.847 | 44.081 | 7.828 | 1.00 | 16.45 | A | C |
| ATOM | 552 | O | ASN | 214 | 111.448 | 43.500 | 8.825 | 1.00 | 17.17 | A | O |
| ATOM | 553 | N | LYS | 215 | 111.080 | 44.289 | 6.764 | 1.00 | 16.88 | A | N |
| ATOM | 554 | CA | LYS | 215 | 109.705 | 43.817 | 6.744 | 1.00 | 17.32 | A | C |
| ATOM | 555 | CB | LYS | 215 | 108.804 | 44.772 | 5.926 | 1.00 | 20.45 | A | C |
| ATOM | 556 | CG | LYS | 215 | 108.670 | 46.176 | 6.531 | 1.00 | 28.03 | A | C |
| ATOM | 557 | CD | LYS | 215 | 107.387 | 46.902 | 6.115 | 1.00 | 31.57 | A | C |
| ATOM | 558 | CE | LYS | 215 | 107.304 | 47.155 | 4.607 | 1.00 | 35.03 | A | C |
| ATOM | 559 | NZ | LYS | 215 | 106.135 | 48.007 | 4.237 | 1.00 | 36.02 | A | N |
| ATOM | 560 | C | LYS | 215 | 109.617 | 42.399 | 6.193 | 1.00 | 15.45 | A | C |
| ATOM | 561 | O | LYS | 215 | 108.529 | 41.825 | 6.124 | 1.00 | 16.67 | A | O |
| ATOM | 562 | N | ILE | 216 | 110.757 | 41.824 | 5.812 | 1.00 | 28.84 | A | N |
| ATOM | 563 | CA | ILE | 216 | 110.754 | 40.475 | 5.262 | 1.00 | 25.66 | A | C |
| ATOM | 564 | CB | ILE | 216 | 112.088 | 40.123 | 4.594 | 1.00 | 13.08 | A | C |
| ATOM | 565 | CG2 | ILE | 216 | 112.088 | 38.681 | 4.163 | 1.00 | 9.86 | A | C |
| ATOM | 566 | CG1 | ILE | 216 | 112.298 | 41.002 | 3.362 | 1.00 | 9.76 | A | C |
| ATOM | 567 | CD1 | ILE | 216 | 113.597 | 40.713 | 2.626 | 1.00 | 6.72 | A | C |
| ATOM | 568 | C | ILE | 216 | 110.459 | 39.445 | 6.333 | 1.00 | 24.10 | A | C |
| ATOM | 569 | O | ILE | 216 | 111.076 | 39.441 | 7.404 | 1.00 | 24.80 | A | O |
| ATOM | 570 | N | VAL | 217 | 109.503 | 38.574 | 6.017 | 1.00 | 14.68 | A | N |
| ATOM | 571 | CA | VAL | 217 | 109.065 | 37.511 | 6.904 | 1.00 | 16.45 | A | C |
| ATOM | 572 | CB | VAL | 217 | 107.535 | 37.425 | 6.901 | 1.00 | 9.81 | A | C |
| ATOM | 573 | CG1 | VAL | 217 | 107.065 | 36.144 | 7.569 | 1.00 | 9.81 | A | C |
| ATOM | 574 | CG2 | VAL | 217 | 106.967 | 38.647 | 7.626 | 1.00 | 9.81 | A | C |
| ATOM | 575 | C | VAL | 217 | 109.641 | 36.173 | 6.483 | 1.00 | 17.61 | A | C |
| ATOM | 576 | O | VAL | 217 | 109.794 | 35.895 | 5.298 | 1.00 | 17.07 | A | O |
| ATOM | 577 | N | GLN | 218 | 109.959 | 35.348 | 7.474 | 1.00 | 15.74 | A | N |
| ATOM | 578 | CA | GLN | 218 | 110.512 | 34.024 | 7.234 | 1.00 | 16.40 | A | C |
| ATOM | 579 | CB | GLN | 218 | 111.064 | 33.446 | 8.531 | 1.00 | 14.26 | A | C |
| ATOM | 580 | CG | GLN | 218 | 111.752 | 32.109 | 8.372 | 1.00 | 14.26 | A | C |
| ATOM | 581 | CD | GLN | 218 | 112.331 | 31.589 | 9.675 | 1.00 | 14.26 | A | C |
| ATOM | 582 | OE1 | GLN | 218 | 113.166 | 30.685 | 9.668 | 1.00 | 14.26 | A | O |
| ATOM | 583 | NE2 | GLN | 218 | 111.887 | 32.156 | 10.802 | 1.00 | 14.26 | A | N |
| ATOM | 584 | C | GLN | 218 | 109.392 | 33.151 | 6.719 | 1.00 | 15.85 | A | C |

Fig. 19: A-9

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 585 | O | GLN | 218 | 108.335 | 33.103 | 7.328 | 1.00 | 19.60 | A | O |
| ATOM | 586 | N | ARG | 219 | 109.622 | 32.464 | 5.604 | 1.00 | 16.04 | A | N |
| ATOM | 587 | CA | ARG | 219 | 108.599 | 31.602 | 5.005 | 1.00 | 15.69 | A | C |
| ATOM | 588 | CB | ARG | 219 | 108.595 | 31.786 | 3.489 | 1.00 | 43.49 | A | C |
| ATOM | 589 | CG | ARG | 219 | 109.053 | 33.163 | 3.054 | 1.00 | 43.49 | A | C |
| ATOM | 590 | CD | ARG | 219 | 108.719 | 33.421 | 1.606 | 1.00 | 43.49 | A | C |
| ATOM | 591 | NE | ARG | 219 | 107.365 | 33.952 | 1.454 | 1.00 | 43.49 | A | N |
| ATOM | 592 | CZ | ARG | 219 | 107.042 | 35.232 | 1.606 | 1.00 | 43.49 | A | C |
| ATOM | 593 | NH1 | ARG | 219 | 107.978 | 36.122 | 1.915 | 1.00 | 43.49 | A | N |
| ATOM | 594 | NH2 | ARG | 219 | 105.786 | 35.621 | 1.443 | 1.00 | 43.49 | A | N |
| ATOM | 595 | C | ARG | 219 | 108.814 | 30.127 | 5.350 | 1.00 | 16.90 | A | C |
| ATOM | 596 | O | ARG | 219 | 108.073 | 29.253 | 4.886 | 1.00 | 16.91 | A | O |
| ATOM | 597 | N | GLY | 220 | 109.838 | 29.867 | 6.160 | 1.00 | 9.58 | A | N |
| ATOM | 598 | CA | GLY | 220 | 110.148 | 28.513 | 6.567 | 1.00 | 9.19 | A | C |
| ATOM | 599 | C | GLY | 220 | 110.442 | 27.562 | 5.422 | 1.00 | 8.86 | A | C |
| ATOM | 600 | O | GLY | 220 | 110.682 | 27.993 | 4.288 | 1.00 | 7.20 | A | O |
| ATOM | 601 | N | GLY | 221 | 110.435 | 26.266 | 5.730 | 1.00 | 16.50 | A | N |
| ATOM | 602 | CA | GLY | 221 | 110.682 | 25.265 | 4.718 | 1.00 | 15.07 | A | C |
| ATOM | 603 | C | GLY | 221 | 111.117 | 23.954 | 5.314 | 1.00 | 15.49 | A | C |
| ATOM | 604 | O | GLY | 221 | 112.038 | 23.928 | 6.124 | 1.00 | 12.29 | A | O |
| ATOM | 605 | N | ARG | 222 | 110.459 | 22.865 | 4.927 | 1.00 | 35.34 | A | N |
| ATOM | 606 | CA | ARG | 222 | 110.815 | 21.543 | 5.433 | 1.00 | 36.05 | A | C |
| ATOM | 607 | CB | ARG | 222 | 109.652 | 20.567 | 5.235 | 1.00 | 22.30 | A | C |
| ATOM | 608 | CG | ARG | 222 | 108.505 | 20.791 | 6.201 | 1.00 | 22.30 | A | C |
| ATOM | 609 | CD | ARG | 222 | 107.252 | 20.047 | 5.779 | 1.00 | 22.30 | A | C |
| ATOM | 610 | NE | ARG | 222 | 106.621 | 20.647 | 4.614 | 1.00 | 22.30 | A | N |
| ATOM | 611 | CZ | ARG | 222 | 105.459 | 20.247 | 4.103 | 1.00 | 22.30 | A | C |
| ATOM | 612 | NH1 | ARG | 222 | 104.795 | 19.241 | 4.654 | 1.00 | 22.30 | A | N |
| ATOM | 613 | NH2 | ARG | 222 | 104.951 | 20.857 | 3.042 | 1.00 | 22.30 | A | N |
| ATOM | 614 | C | ARG | 222 | 112.062 | 21.036 | 4.723 | 1.00 | 36.10 | A | C |
| ATOM | 615 | O | ARG | 222 | 112.626 | 20.017 | 5.107 | 1.00 | 36.87 | A | O |
| ATOM | 616 | N | GLN | 223 | 112.473 | 21.750 | 3.678 | 1.00 | 27.48 | A | N |
| ATOM | 617 | CA | GLN | 223 | 113.672 | 21.428 | 2.912 | 1.00 | 25.77 | A | C |
| ATOM | 618 | CB | GLN | 223 | 113.328 | 20.858 | 1.535 | 1.00 | 13.17 | A | C |
| ATOM | 619 | CG | GLN | 223 | 112.830 | 19.417 | 1.508 | 1.00 | 14.61 | A | C |
| ATOM | 620 | CD | GLN | 223 | 111.346 | 19.312 | 1.790 | 1.00 | 15.02 | A | C |
| ATOM | 621 | OE1 | GLN | 223 | 110.533 | 20.016 | 1.190 | 1.00 | 15.42 | A | O |
| ATOM | 622 | NE2 | GLN | 223 | 110.981 | 18.417 | 2.698 | 1.00 | 15.46 | A | N |
| ATOM | 623 | C | GLN | 223 | 114.498 | 22.706 | 2.724 | 1.00 | 26.51 | A | C |
| ATOM | 624 | O | GLN | 223 | 114.057 | 23.799 | 3.069 | 1.00 | 25.99 | A | O |
| ATOM | 625 | N | THR | 224 | 115.696 | 22.567 | 2.172 | 1.00 | 24.40 | A | N |
| ATOM | 626 | CA | THR | 224 | 116.581 | 23.704 | 1.948 | 1.00 | 22.28 | A | C |
| ATOM | 627 | CB | THR | 224 | 117.795 | 23.633 | 2.897 | 1.00 | 14.98 | A | C |
| ATOM | 628 | OG1 | THR | 224 | 117.328 | 23.565 | 4.246 | 1.00 | 14.97 | A | O |
| ATOM | 629 | CG2 | THR | 224 | 118.683 | 24.849 | 2.747 | 1.00 | 11.28 | A | C |
| ATOM | 630 | C | THR | 224 | 117.061 | 23.662 | 0.500 | 1.00 | 19.29 | A | C |
| ATOM | 631 | O | THR | 224 | 118.122 | 23.129 | 0.202 | 1.00 | 15.78 | A | O |
| ATOM | 632 | N | MET | 225 | 116.272 | 24.234 | -0.395 | 1.00 | 14.15 | A | N |
| ATOM | 633 | CA | MET | 225 | 116.607 | 24.236 | -1.810 | 1.00 | 15.04 | A | C |
| ATOM | 634 | CB | MET | 225 | 115.346 | 24.481 | -2.636 | 1.00 | 22.98 | A | C |
| ATOM | 635 | CG | MET | 225 | 114.183 | 23.602 | -2.267 | 1.00 | 20.41 | A | C |
| ATOM | 636 | SD | MET | 225 | 114.421 | 21.883 | -2.704 | 1.00 | 28.15 | A | S |
| ATOM | 637 | CE | MET | 225 | 112.675 | 21.302 | -2.554 | 1.00 | 24.73 | A | C |
| ATOM | 638 | C | MET | 225 | 117.653 | 25.275 | -2.204 | 1.00 | 16.07 | A | C |
| ATOM | 639 | O | MET | 225 | 117.426 | 26.054 | -3.136 | 1.00 | 17.53 | A | O |
| ATOM | 640 | N | THR | 226 | 118.791 | 25.297 | -1.513 | 1.00 | 16.19 | A | N |
| ATOM | 641 | CA | THR | 226 | 119.841 | 26.259 | -1.840 | 1.00 | 15.66 | A | C |
| ATOM | 642 | CB | THR | 226 | 121.155 | 25.905 | -1.129 | 1.00 | 25.30 | A | C |
| ATOM | 643 | OG1 | THR | 226 | 120.925 | 25.825 | 0.284 | 1.00 | 27.32 | A | O |
| ATOM | 644 | CG2 | THR | 226 | 122.216 | 26.959 | -1.414 | 1.00 | 23.02 | A | C |
| ATOM | 645 | C | THR | 226 | 120.100 | 26.337 | -3.356 | 1.00 | 14.26 | A | C |
| ATOM | 646 | O | THR | 226 | 120.229 | 27.418 | -3.917 | 1.00 | 8.95 | A | O |
| ATOM | 647 | N | ALA | 227 | 120.158 | 25.190 | -4.019 | 1.00 | 9.41 | A | N |
| ATOM | 648 | CA | ALA | 227 | 120.408 | 25.162 | -5.448 | 1.00 | 8.35 | A | C |
| ATOM | 649 | CB | ALA | 227 | 120.422 | 23.738 | -5.939 | 1.00 | 23.80 | A | C |
| ATOM | 650 | C | ALA | 227 | 119.342 | 25.951 | -6.188 | 1.00 | 9.01 | A | C |
| ATOM | 651 | O | ALA | 227 | 119.644 | 26.759 | -7.067 | 1.00 | 9.81 | A | O |
| ATOM | 652 | N | LEU | 228 | 118.085 | 25.711 | -5.842 | 1.00 | 28.18 | A | N |
| ATOM | 653 | CA | LEU | 228 | 116.985 | 26.410 | -6.489 | 1.00 | 26.62 | A | C |
| ATOM | 654 | CB | LEU | 228 | 115.649 | 25.860 | -5.988 | 1.00 | 14.81 | A | C |
| ATOM | 655 | CG | LEU | 228 | 114.372 | 26.485 | -6.557 | 1.00 | 22.70 | A | C |
| ATOM | 656 | CD1 | LEU | 228 | 114.356 | 26.363 | -8.080 | 1.00 | 20.29 | A | C |
| ATOM | 657 | CD2 | LEU | 228 | 113.163 | 25.801 | -5.947 | 1.00 | 19.75 | A | C |

# Fig. 19: A-10

```
ATOM    658  C   LEU   228     117.067  27.909  -6.221  1.00   25.80      A    C
ATOM    659  O   LEU   228     116.885  28.719  -7.129  1.00   28.78      A    O
ATOM    660  N   GLY   229     117.341  28.274  -4.971  1.00   23.50      A    N
ATOM    661  CA  GLY   229     117.449  29.679  -4.624  1.00   25.86      A    C
ATOM    662  C   GLY   229     118.464  30.407  -5.495  1.00   28.42      A    C
ATOM    663  O   GLY   229     118.149  31.428  -6.108  1.00   29.01      A    O
ATOM    664  N   ILE   230     119.682  29.876  -5.562  1.00   20.49      A    N
ATOM    665  CA  ILE   230     120.736  30.498  -6.354  1.00   21.82      A    C
ATOM    666  CB  ILE   230     122.096  29.779  -6.195  1.00    2.66      A    C
ATOM    667  CG2 ILE   230     123.168  30.546  -6.953  1.00    2.66      A    C
ATOM    668  CG1 ILE   230     122.486  29.692  -4.720  1.00    2.66      A    C
ATOM    669  CD1 ILE   230     123.773  28.920  -4.474  1.00    2.66      A    C
ATOM    670  C   ILE   230     120.386  30.508  -7.830  1.00   22.08      A    C
ATOM    671  O   ILE   230     120.614  31.498  -8.511  1.00   20.01      A    O
ATOM    672  N   ASP   231     119.841  29.409  -8.333  1.00   32.19      A    N
ATOM    673  CA  ASP   231     119.473  29.352  -9.743  1.00   30.59      A    C
ATOM    674  CB  ASP   231     118.959  27.958 -10.103  1.00   35.41      A    C
ATOM    675  CG  ASP   231     118.860  27.739 -11.604  1.00   42.41      A    C
ATOM    676  OD1 ASP   231     119.910  27.778 -12.281  1.00   41.17      A    O
ATOM    677  OD2 ASP   231     117.735  27.525 -12.103  1.00   45.95      A    O
ATOM    678  C   ASP   231     118.392  30.395 -10.048  1.00   31.57      A    C
ATOM    679  O   ASP   231     118.429  31.048 -11.090  1.00   28.79      A    O
ATOM    680  N   THR   232     117.443  30.554  -9.126  1.00   18.29      A    N
ATOM    681  CA  THR   232     116.347  31.510  -9.296  1.00   17.08      A    C
ATOM    682  CB  THR   232     115.287  31.347  -8.194  1.00   20.70      A    C
ATOM    683  OG1 THR   232     114.714  30.041  -8.279  1.00   19.21      A    O
ATOM    684  CG2 THR   232     114.191  32.370  -8.358  1.00   14.24      A    C
ATOM    685  C   THR   232     116.859  32.937  -9.264  1.00   17.71      A    C
ATOM    686  O   THR   232     116.390  33.801 -10.010  1.00   17.88      A    O
ATOM    687  N   ALA   233     117.815  33.187  -8.379  1.00   19.66      A    N
ATOM    688  CA  ALA   233     118.395  34.517  -8.270  1.00   22.31      A    C
ATOM    689  CB  ALA   233     119.364  34.580  -7.099  1.00   15.15      A    C
ATOM    690  C   ALA   233     119.125  34.796  -9.575  1.00   24.62      A    C
ATOM    691  O   ALA   233     119.187  35.929 -10.031  1.00   26.53      A    O
ATOM    692  N   ARG   234     119.666  33.746 -10.180  1.00   30.19      A    N
ATOM    693  CA  ARG   234     120.390  33.879 -11.434  1.00   33.29      A    C
ATOM    694  CB  ARG   234     121.241  32.637 -11.693  1.00   15.32      A    C
ATOM    695  CG  ARG   234     122.345  32.875 -12.693  1.00   15.32      A    C
ATOM    696  CD  ARG   234     122.760  31.617 -13.460  1.00   15.32      A    C
ATOM    697  NE  ARG   234     121.839  31.311 -14.554  1.00   15.32      A    N
ATOM    698  CZ  ARG   234     120.875  30.405 -14.481  1.00   15.32      A    C
ATOM    699  NH1 ARG   234     120.708  29.713 -13.368  1.00   15.32      A    N
ATOM    700  NH2 ARG   234     120.078  30.188 -15.511  1.00   15.32      A    N
ATOM    701  C   ARG   234     119.446  34.083 -12.619  1.00   35.42      A    C
ATOM    702  O   ARG   234     119.409  35.153 -13.215  1.00   35.47      A    O
ATOM    703  N   LYS   235     118.666  33.057 -12.941  1.00   67.48      A    N
ATOM    704  CA  LYS   235     117.767  33.124 -14.085  1.00   67.43      A    C
ATOM    705  CB  LYS   235     117.204  31.730 -14.397  1.00   53.18      A    C
ATOM    706  CG  LYS   235     115.965  31.308 -13.615  1.00   54.33      A    C
ATOM    707  CD  LYS   235     115.583  29.867 -13.970  1.00   54.15      A    C
ATOM    708  CE  LYS   235     114.146  29.517 -13.590  1.00   54.95      A    C
ATOM    709  NZ  LYS   235     113.873  29.660 -12.135  1.00   55.71      A    N
ATOM    710  C   LYS   235     116.628  34.134 -14.017  1.00   67.57      A    C
ATOM    711  O   LYS   235     116.074  34.500 -15.054  1.00   67.91      A    O
ATOM    712  N   GLU   236     116.277  34.596 -12.822  1.00   98.68      A    N
ATOM    713  CA  GLU   236     115.186  35.558 -12.693  1.00  100.30      A    C
ATOM    714  CB  GLU   236     114.087  34.999 -11.781  1.00   50.64      A    C
ATOM    715  CG  GLU   236     113.008  34.192 -12.510  1.00   53.41      A    C
ATOM    716  CD  GLU   236     112.199  33.276 -11.582  1.00   55.89      A    C
ATOM    717  OE1 GLU   236     111.660  33.760 -10.565  1.00   55.98      A    O
ATOM    718  OE2 GLU   236     112.098  32.065 -11.875  1.00   55.73      A    O
ATOM    719  C   GLU   236     115.627  36.917 -12.174  1.00   98.85      A    C
ATOM    720  O   GLU   236     115.638  37.900 -12.912  1.00  100.28      A    O
ATOM    721  N   ALA   237     115.991  36.969 -10.899  1.00   71.25      A    N
ATOM    722  CA  ALA   237     116.405  38.218 -10.276  1.00   68.72      A    C
ATOM    723  CB  ALA   237     117.046  37.934  -8.932  1.00   56.85      A    C
ATOM    724  C   ALA   237     117.349  39.046 -11.139  1.00   67.56      A    C
ATOM    725  O   ALA   237     117.225  40.267 -11.200  1.00   65.98      A    O
ATOM    726  N   PHE   238     118.283  38.385 -11.812  1.00   41.81      A    N
ATOM    727  CA  PHE   238     119.256  39.080 -12.651  1.00   41.24      A    C
ATOM    728  CB  PHE   238     120.606  38.369 -12.591  1.00   47.57      A    C
ATOM    729  CG  PHE   238     121.413  38.696 -11.378  1.00   46.60      A    C
ATOM    730  CD1 PHE   238     121.686  37.725 -10.419  1.00   47.83      A    C
```

Fig. 19: A-11

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 731 | CD2 | PHE | 238 | 121.931 | 39.970 | -11.208 | 1.00 | 44.20 | A | C |
| ATOM | 732 | CE1 | PHE | 238 | 122.476 | 38.023 | -9.298 | 1.00 | 45.63 | A | C |
| ATOM | 733 | CE2 | PHE | 238 | 122.719 | 40.282 | -10.094 | 1.00 | 50.51 | A | C |
| ATOM | 734 | CZ | PHE | 238 | 122.993 | 39.305 | -9.137 | 1.00 | 51.93 | A | C |
| ATOM | 735 | C | PHE | 238 | 118.861 | 39.252 | -14.116 | 1.00 | 43.09 | A | C |
| ATOM | 736 | O | PHE | 238 | 119.699 | 39.129 | -15.017 | 1.00 | 43.19 | A | O |
| ATOM | 737 | N | THR | 239 | 117.586 | 39.520 | -14.362 | 1.00 | 28.84 | A | N |
| ATOM | 738 | CA | THR | 239 | 117.117 | 39.744 | -15.724 | 1.00 | 32.78 | A | C |
| ATOM | 739 | CB | THR | 239 | 115.952 | 38.821 | -16.086 | 1.00 | 22.29 | A | C |
| ATOM | 740 | OG1 | THR | 239 | 114.866 | 39.059 | -15.191 | 1.00 | 20.25 | A | O |
| ATOM | 741 | CG2 | THR | 239 | 116.363 | 37.382 | -15.988 | 1.00 | 25.20 | A | C |
| ATOM | 742 | C | THR | 239 | 116.655 | 41.202 | -15.798 | 1.00 | 33.04 | A | C |
| ATOM | 743 | O | THR | 239 | 115.955 | 41.695 | -14.902 | 1.00 | 33.54 | A | O |
| ATOM | 744 | N | GLU | 240 | 117.067 | 41.881 | -16.868 | 1.00 | 73.11 | A | N |
| ATOM | 745 | CA | GLU | 240 | 116.755 | 43.291 | -17.085 | 1.00 | 73.36 | A | C |
| ATOM | 746 | CB | GLU | 240 | 116.995 | 43.654 | -18.549 | 1.00 | 97.49 | A | C |
| ATOM | 747 | CG | GLU | 240 | 117.147 | 45.141 | -18.793 | 1.00 | 102.13 | A | C |
| ATOM | 748 | CD | GLU | 240 | 117.738 | 45.441 | -20.152 | 1.00 | 105.04 | A | C |
| ATOM | 749 | OE1 | GLU | 240 | 118.794 | 44.858 | -20.483 | 1.00 | 105.14 | A | O |
| ATOM | 750 | OE2 | GLU | 240 | 117.151 | 46.263 | -20.885 | 1.00 | 105.11 | A | O |
| ATOM | 751 | C | GLU | 240 | 115.336 | 43.665 | -16.689 | 1.00 | 74.71 | A | C |
| ATOM | 752 | O | GLU | 240 | 115.083 | 44.772 | -16.210 | 1.00 | 75.92 | A | O |
| ATOM | 753 | N | ALA | 241 | 114.417 | 42.730 | -16.885 | 1.00 | 32.59 | A | N |
| ATOM | 754 | CA | ALA | 241 | 113.016 | 42.952 | -16.552 | 1.00 | 33.44 | A | C |
| ATOM | 755 | CB | ALA | 241 | 112.170 | 41.769 | -17.051 | 1.00 | 4.05 | A | C |
| ATOM | 756 | C | ALA | 241 | 112.802 | 43.165 | -15.044 | 1.00 | 32.91 | A | C |
| ATOM | 757 | O | ALA | 241 | 111.809 | 43.759 | -14.622 | 1.00 | 34.37 | A | O |
| ATOM | 758 | N | ARG | 242 | 113.725 | 42.678 | -14.223 | 1.00 | 31.60 | A | N |
| ATOM | 759 | CA | ARG | 242 | 113.585 | 42.851 | -12.786 | 1.00 | 31.34 | A | C |
| ATOM | 760 | CB | ARG | 242 | 113.757 | 41.500 | -12.079 | 1.00 | 27.81 | A | C |
| ATOM | 761 | CG | ARG | 242 | 112.489 | 40.658 | -12.052 | 1.00 | 28.01 | A | C |
| ATOM | 762 | CD | ARG | 242 | 112.669 | 39.440 | -11.160 | 1.00 | 28.87 | A | C |
| ATOM | 763 | NE | ARG | 242 | 111.425 | 39.010 | -10.515 | 1.00 | 30.07 | A | N |
| ATOM | 764 | CZ | ARG | 242 | 110.582 | 38.106 | -11.011 | 1.00 | 29.27 | A | C |
| ATOM | 765 | NH1 | ARG | 242 | 110.846 | 37.525 | -12.176 | 1.00 | 28.32 | A | N |
| ATOM | 766 | NH2 | ARG | 242 | 109.485 | 37.769 | -10.334 | 1.00 | 31.29 | A | N |
| ATOM | 767 | C | ARG | 242 | 114.557 | 43.898 | -12.231 | 1.00 | 32.54 | A | C |
| ATOM | 768 | O | ARG | 242 | 114.824 | 43.954 | -11.026 | 1.00 | 35.55 | A | O |
| ATOM | 769 | N | GLY | 243 | 115.080 | 44.733 | -13.122 | 1.00 | 38.70 | A | N |
| ATOM | 770 | CA | GLY | 243 | 115.996 | 45.775 | -12.706 | 1.00 | 36.85 | A | C |
| ATOM | 771 | C | GLY | 243 | 117.468 | 45.462 | -12.890 | 1.00 | 35.13 | A | C |
| ATOM | 772 | O | GLY | 243 | 118.318 | 46.139 | -12.308 | 1.00 | 34.75 | A | O |
| ATOM | 773 | N | ALA | 244 | 117.792 | 44.447 | -13.683 | 1.00 | 32.25 | A | N |
| ATOM | 774 | CA | ALA | 244 | 119.190 | 44.119 | -13.896 | 1.00 | 30.25 | A | C |
| ATOM | 775 | CB | ALA | 244 | 119.326 | 42.709 | -14.442 | 1.00 | 67.28 | A | C |
| ATOM | 776 | C | ALA | 244 | 119.750 | 45.130 | -14.886 | 1.00 | 32.13 | A | C |
| ATOM | 777 | O | ALA | 244 | 119.437 | 45.088 | -16.068 | 1.00 | 31.59 | A | O |
| ATOM | 778 | N | ARG | 245 | 120.566 | 46.054 | -14.401 | 1.00 | 18.96 | A | N |
| ATOM | 779 | CA | ARG | 245 | 121.154 | 47.074 | -15.258 | 1.00 | 19.79 | A | C |
| ATOM | 780 | CB | ARG | 245 | 121.853 | 48.130 | -14.399 | 1.00 | 36.60 | A | C |
| ATOM | 781 | CG | ARG | 245 | 120.888 | 49.043 | -13.655 | 1.00 | 39.07 | A | C |
| ATOM | 782 | CD | ARG | 245 | 121.614 | 49.991 | -12.741 | 1.00 | 39.28 | A | C |
| ATOM | 783 | NE | ARG | 245 | 122.309 | 49.254 | -11.701 | 1.00 | 33.70 | A | N |
| ATOM | 784 | CZ | ARG | 245 | 122.997 | 49.824 | -10.726 | 1.00 | 33.52 | A | C |
| ATOM | 785 | NH1 | ARG | 245 | 123.084 | 51.145 | -10.662 | 1.00 | 32.72 | A | N |
| ATOM | 786 | NH2 | ARG | 245 | 123.590 | 49.075 | -9.810 | 1.00 | 30.81 | A | N |
| ATOM | 787 | C | ARG | 245 | 122.131 | 46.493 | -16.266 | 1.00 | 18.16 | A | C |
| ATOM | 788 | O | ARG | 245 | 123.003 | 45.710 | -15.911 | 1.00 | 14.27 | A | O |
| ATOM | 789 | N | ARG | 246 | 121.985 | 46.896 | -17.525 | 1.00 | 55.16 | A | N |
| ATOM | 790 | CA | ARG | 246 | 122.848 | 46.429 | -18.607 | 1.00 | 57.95 | A | C |
| ATOM | 791 | CB | ARG | 246 | 122.447 | 47.078 | -19.928 | 1.00 | 115.62 | A | C |
| ATOM | 792 | CG | ARG | 246 | 123.405 | 46.764 | -21.067 | 1.00 | 120.98 | A | C |
| ATOM | 793 | CD | ARG | 246 | 123.057 | 47.546 | -22.318 | 1.00 | 126.90 | A | C |
| ATOM | 794 | NE | ARG | 246 | 121.637 | 47.444 | -22.641 | 1.00 | 129.81 | A | N |
| ATOM | 795 | CZ | ARG | 246 | 120.981 | 46.298 | -22.804 | 1.00 | 132.92 | A | C |
| ATOM | 796 | NH1 | ARG | 246 | 121.615 | 45.138 | -22.676 | 1.00 | 132.61 | A | N |
| ATOM | 797 | NH2 | ARG | 246 | 119.685 | 46.314 | -23.094 | 1.00 | 133.70 | A | N |
| ATOM | 798 | C | ARG | 246 | 124.313 | 46.736 | -18.364 | 1.00 | 55.77 | A | C |
| ATOM | 799 | O | ARG | 246 | 124.671 | 47.879 | -18.092 | 1.00 | 58.40 | A | O |
| ATOM | 800 | N | GLY | 247 | 125.151 | 45.711 | -18.475 | 1.00 | 47.75 | A | N |
| ATOM | 801 | CA | GLY | 247 | 126.587 | 45.878 | -18.302 | 1.00 | 50.33 | A | C |
| ATOM | 802 | C | GLY | 247 | 127.097 | 46.294 | -16.934 | 1.00 | 50.40 | A | C |
| ATOM | 803 | O | GLY | 247 | 128.129 | 46.958 | -16.824 | 1.00 | 53.36 | A | O |

Fig. 19: A-12

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 804 | N | VAL | 248 | 126.382 | 45.911 | -15.887 | 1.00 | 40.38 | A | N |
| ATOM | 805 | CA | VAL | 248 | 126.790 | 46.248 | -14.535 | 1.00 | 38.39 | A | C |
| ATOM | 806 | CB | VAL | 248 | 125.653 | 46.928 | -13.780 | 1.00 | 41.70 | A | C |
| ATOM | 807 | CG1 | VAL | 248 | 126.049 | 47.136 | -12.331 | 1.00 | 39.35 | A | C |
| ATOM | 808 | CG2 | VAL | 248 | 125.331 | 48.250 | -14.436 | 1.00 | 33.47 | A | C |
| ATOM | 809 | C | VAL | 248 | 127.173 | 44.970 | -13.807 | 1.00 | 41.41 | A | C |
| ATOM | 810 | O | VAL | 248 | 126.530 | 43.936 | -13.993 | 1.00 | 45.46 | A | O |
| ATOM | 811 | N | LYS | 249 | 128.208 | 45.036 | -12.975 | 1.00 | 30.45 | A | N |
| ATOM | 812 | CA | LYS | 249 | 128.645 | 43.852 | -12.250 | 1.00 | 31.36 | A | C |
| ATOM | 813 | CB | LYS | 249 | 129.799 | 44.186 | -11.299 | 1.00 | 85.59 | A | C |
| ATOM | 814 | CG | LYS | 249 | 130.426 | 42.940 | -10.690 | 1.00 | 91.11 | A | C |
| ATOM | 815 | CD | LYS | 249 | 130.844 | 41.943 | -11.782 | 1.00 | 92.18 | A | C |
| ATOM | 816 | CE | LYS | 249 | 131.040 | 40.539 | -11.224 | 1.00 | 94.54 | A | C |
| ATOM | 817 | NZ | LYS | 249 | 131.548 | 39.546 | -12.218 | 1.00 | 97.36 | A | N |
| ATOM | 818 | C | LYS | 249 | 127.503 | 43.190 | -11.473 | 1.00 | 30.02 | A | C |
| ATOM | 819 | O | LYS | 249 | 126.706 | 43.862 | -10.815 | 1.00 | 29.84 | A | O |
| ATOM | 820 | N | LYS | 250 | 127.432 | 41.864 | -11.559 | 1.00 | 29.51 | A | N |
| ATOM | 821 | CA | LYS | 250 | 126.396 | 41.110 | -10.879 | 1.00 | 29.16 | A | C |
| ATOM | 822 | CB | LYS | 250 | 125.763 | 40.134 | -11.871 | 1.00 | 45.59 | A | C |
| ATOM | 823 | CG | LYS | 250 | 125.050 | 40.864 | -12.996 | 1.00 | 44.19 | A | C |
| ATOM | 824 | CD | LYS | 250 | 124.892 | 40.022 | -14.263 | 1.00 | 45.74 | A | C |
| ATOM | 825 | CE | LYS | 250 | 123.827 | 38.928 | -14.135 | 1.00 | 44.90 | A | C |
| ATOM | 826 | NZ | LYS | 250 | 123.513 | 38.274 | -15.453 | 1.00 | 46.72 | A | N |
| ATOM | 827 | C | LYS | 250 | 126.979 | 40.391 | -9.663 | 1.00 | 28.51 | A | C |
| ATOM | 828 | O | LYS | 250 | 127.849 | 39.541 | -9.804 | 1.00 | 28.19 | A | O |
| ATOM | 829 | N | VAL | 251 | 126.493 | 40.754 | -8.474 | 1.00 | 23.05 | A | N |
| ATOM | 830 | CA | VAL | 251 | 126.954 | 40.173 | -7.219 | 1.00 | 22.96 | A | C |
| ATOM | 831 | CB | VAL | 251 | 127.504 | 41.263 | -6.307 | 1.00 | 28.85 | A | C |
| ATOM | 832 | CG1 | VAL | 251 | 127.901 | 40.676 | -4.959 | 1.00 | 27.00 | A | C |
| ATOM | 833 | CG2 | VAL | 251 | 128.678 | 41.928 | -6.974 | 1.00 | 30.06 | A | C |
| ATOM | 834 | C | VAL | 251 | 125.863 | 39.421 | -6.451 | 1.00 | 21.44 | A | C |
| ATOM | 835 | O | VAL | 251 | 124.778 | 39.945 | -6.232 | 1.00 | 17.44 | A | O |
| ATOM | 836 | N | MET | 252 | 126.168 | 38.199 | -6.023 | 1.00 | 19.32 | A | N |
| ATOM | 837 | CA | MET | 252 | 125.212 | 37.383 | -5.278 | 1.00 | 20.30 | A | C |
| ATOM | 838 | CB | MET | 252 | 124.949 | 36.073 | -6.024 | 1.00 | 19.49 | A | C |
| ATOM | 839 | CG | MET | 252 | 123.850 | 35.212 | -5.425 | 1.00 | 18.18 | A | C |
| ATOM | 840 | SD | MET | 252 | 123.556 | 33.701 | -6.379 | 1.00 | 22.23 | A | S |
| ATOM | 841 | CE | MET | 252 | 123.009 | 34.366 | -7.960 | 1.00 | 13.54 | A | C |
| ATOM | 842 | C | MET | 252 | 125.730 | 37.072 | -3.875 | 1.00 | 19.32 | A | C |
| ATOM | 843 | O | MET | 252 | 126.880 | 36.675 | -3.704 | 1.00 | 21.69 | A | O |
| ATOM | 844 | N | VAL | 253 | 124.886 | 37.261 | -2.869 | 1.00 | 11.70 | A | N |
| ATOM | 845 | CA | VAL | 253 | 125.286 | 36.971 | -1.505 | 1.00 | 12.85 | A | C |
| ATOM | 846 | CB | VAL | 253 | 125.173 | 38.221 | -0.593 | 1.00 | 5.67 | A | C |
| ATOM | 847 | CG1 | VAL | 253 | 125.508 | 37.856 | 0.842 | 1.00 | 7.09 | A | C |
| ATOM | 848 | CG2 | VAL | 253 | 126.118 | 39.310 | -1.079 | 1.00 | 5.31 | A | C |
| ATOM | 849 | C | VAL | 253 | 124.370 | 35.881 | -0.974 | 1.00 | 12.42 | A | C |
| ATOM | 850 | O | VAL | 253 | 123.166 | 36.093 | -0.870 | 1.00 | 10.86 | A | O |
| ATOM | 851 | N | ILE | 254 | 124.936 | 34.716 | -0.649 | 1.00 | 26.88 | A | N |
| ATOM | 852 | CA | ILE | 254 | 124.142 | 33.597 | -0.126 | 1.00 | 23.78 | A | C |
| ATOM | 853 | CB | ILE | 254 | 124.457 | 32.266 | -0.847 | 1.00 | 10.72 | A | C |
| ATOM | 854 | CG2 | ILE | 254 | 123.584 | 31.171 | -0.294 | 1.00 | 7.19 | A | C |
| ATOM | 855 | CG1 | ILE | 254 | 124.220 | 32.397 | -2.352 | 1.00 | 9.30 | A | C |
| ATOM | 856 | CD1 | ILE | 254 | 125.307 | 33.140 | -3.078 | 1.00 | 8.93 | A | C |
| ATOM | 857 | C | ILE | 254 | 124.379 | 33.370 | 1.359 | 1.00 | 21.87 | A | C |
| ATOM | 858 | O | ILE | 254 | 125.508 | 33.431 | 1.833 | 1.00 | 23:74 | A | O |
| ATOM | 859 | N | VAL | 255 | 123.300 | 33.105 | 2.084 | 1.00 | 38.19 | A | N |
| ATOM | 860 | CA | VAL | 255 | 123.379 | 32.858 | 3.516 | 1.00 | 36.93 | A | C |
| ATOM | 861 | CB | VAL | 255 | 122.733 | 33.994 | 4.328 | 1.00 | 13.80 | A | C |
| ATOM | 862 | CG1 | VAL | 255 | 123.224 | 33.949 | 5.753 | 1.00 | 12.25 | A | C |
| ATOM | 863 | CG2 | VAL | 255 | 123.056 | 35.325 | 3.713 | 1.00 | 14.44 | A | C |
| ATOM | 864 | C | VAL | 255 | 122.592 | 31.594 | 3.798 | 1.00 | 34.68 | A | C |
| ATOM | 865 | O | VAL | 255 | 121.431 | 31.491 | 3.403 | 1.00 | 36.68 | A | O |
| ATOM | 866 | N | THR | 256 | 123.210 | 30.632 | 4.474 | 1.00 | 19.22 | A | N |
| ATOM | 867 | CA | THR | 256 | 122.514 | 29.387 | 4.798 | 1.00 | 20.04 | A | C |
| ATOM | 868 | CB | THR | 256 | 122.477 | 28.457 | 3.566 | 1.00 | 10.08 | A | C |
| ATOM | 869 | OG1 | THR | 256 | 122.032 | 27.147 | 3.952 | 1.00 | 6.12 | A | O |
| ATOM | 870 | CG2 | THR | 256 | 123.851 | 28.387 | 2.926 | 1.00 | 8.93 | A | C |
| ATOM | 871 | C | THR | 256 | 123.128 | 28.650 | 5.995 | 1.00 | 23.52 | A | C |
| ATOM | 872 | O | THR | 256 | 124.303 | 28.831 | 6.310 | 1.00 | 19.68 | A | O |
| ATOM | 873 | N | ASP | 257 | 122.323 | 27.829 | 6.663 | 1.00 | 46.58 | A | N |
| ATOM | 874 | CA | ASP | 257 | 122.794 | 27.097 | 7.830 | 1.00 | 46.96 | A | C |
| ATOM | 875 | CB | ASP | 257 | 122.069 | 27.585 | 9.091 | 1.00 | 21.89 | A | C |
| ATOM | 876 | CG | ASP | 257 | 120.655 | 27.009 | 9.225 | 1.00 | 27.25 | A | C |

Fig. 19: A-13

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 877 | OD1 | ASP | 257 | 120.089 | 26.573 | 8.191 | 1.00 | 27.72 | A | O |
| ATOM | 878 | OD2 | ASP | 257 | 120.110 | 27.006 | 10.362 | 1.00 | 32.52 | A | O |
| ATOM | 879 | C | ASP | 257 | 122.599 | 25.596 | 7.693 | 1.00 | 43.55 | A | C |
| ATOM | 880 | O | ASP | 257 | 122.525 | 24.883 | 8.695 | 1.00 | 42.79 | A | O |
| ATOM | 881 | N | GLY | 258 | 122.510 | 25.106 | 6.461 | 1.00 | 42.38 | A | N |
| ATOM | 882 | CA | GLY | 258 | 122.330 | 23.678 | 6.283 | 1.00 | 44.80 | A | C |
| ATOM | 883 | C | GLY | 258 | 122.618 | 23.150 | 4.896 | 1.00 | 48.62 | A | C |
| ATOM | 884 | O | GLY | 258 | 122.523 | 23.871 | 3.903 | 1.00 | 44.34 | A | O |
| ATOM | 885 | N | GLU | 259 | 122.984 | 21.876 | 4.832 | 1.00 | 88.78 | A | N |
| ATOM | 886 | CA | GLU | 259 | 123.265 | 21.230 | 3.562 | 1.00 | 90.66 | A | C |
| ATOM | 887 | CB | GLU | 259 | 123.650 | 19.770 | 3.782 | 1.00 | 87.02 | A | C |
| ATOM | 888 | CG | GLU | 259 | 124.983 | 19.588 | 4.461 | 1.00 | 94.80 | A | C |
| ATOM | 889 | CD | GLU | 259 | 125.130 | 18.214 | 5.070 | 1.00 | 98.61 | A | C |
| ATOM | 890 | OE1 | GLU | 259 | 126.256 | 17.861 | 5.481 | 1.00 | 105.36 | A | O |
| ATOM | 891 | OE2 | GLU | 259 | 124.115 | 17.490 | 5.147 | 1.00 | 98.63 | A | O |
| ATOM | 892 | C | GLU | 259 | 122.004 | 21.298 | 2.727 | 1.00 | 89.52 | A | C |
| ATOM | 893 | O | GLU | 259 | 120.927 | 20.906 | 3.174 | 1.00 | 86.69 | A | O |
| ATOM | 894 | N | SER | 260 | 122.140 | 21.815 | 1.517 | 1.00 | 31.72 | A | N |
| ATOM | 895 | CA | SER | 260 | 121.007 | 21.922 | 0.615 | 1.00 | 34.88 | A | C |
| ATOM | 896 | CB | SER | 260 | 121.435 | 22.606 | -0.685 | 1.00 | 104.64 | A | C |
| ATOM | 897 | OG | SER | 260 | 122.467 | 21.872 | -1.325 | 1.00 | 105.15 | A | O |
| ATOM | 898 | C | SER | 260 | 120.489 | 20.526 | 0.304 | 1.00 | 34.78 | A | C |
| ATOM | 899 | O | SER | 260 | 121.257 | 19.571 | 0.315 | 1.00 | 30.81 | A | O |
| ATOM | 900 | N | HIS | 261 | 119.192 | 20.409 | 0.039 | 1.00 | 119.42 | A | N |
| ATOM | 901 | CA | HIS | 261 | 118.609 | 19.114 | -0.284 | 1.00 | 123.77 | A | C |
| ATOM | 902 | CB | HIS | 261 | 117.107 | 19.116 | 0.020 | 1.00 | 89.56 | A | C |
| ATOM | 903 | CG | HIS | 261 | 116.789 | 19.030 | 1.482 | 1.00 | 92.76 | A | C |
| ATOM | 904 | CD2 | HIS | 261 | 116.610 | 19.997 | 2.413 | 1.00 | 91.87 | A | C |
| ATOM | 905 | ND1 | HIS | 261 | 116.648 | 17.830 | 2.147 | 1.00 | 94.24 | A | N |
| ATOM | 906 | CE1 | HIS | 261 | 116.393 | 18.065 | 3.422 | 1.00 | 94.31 | A | C |
| ATOM | 907 | NE2 | HIS | 261 | 116.365 | 19.372 | 3.610 | 1.00 | 91.58 | A | N |
| ATOM | 908 | C | HIS | 261 | 118.866 | 18.815 | -1.754 | 1.00 | 124.83 | A | C |
| ATOM | 909 | O | HIS | 261 | 118.732 | 17.676 | -2.203 | 1.00 | 122.05 | A | O |
| ATOM | 910 | N | ASP | 262 | 119.251 | 19.850 | -2.495 | 1.00 | 94.20 | A | N |
| ATOM | 911 | CA | ASP | 262 | 119.556 | 19.709 | -3.913 | 1.00 | 99.17 | A | C |
| ATOM | 912 | CB | ASP | 262 | 118.838 | 20.798 | -4.732 | 1.00 | 77.35 | A | C |
| ATOM | 913 | CG | ASP | 262 | 118.558 | 22.065 | -3.929 | 1.00 | 77.35 | A | C |
| ATOM | 914 | OD1 | ASP | 262 | 119.382 | 22.429 | -3.067 | 1.00 | 77.35 | A | O |
| ATOM | 915 | OD2 | ASP | 262 | 117.515 | 22.708 | -4.179 | 1.00 | 77.35 | A | O |
| ATOM | 916 | C | ASP | 262 | 121.065 | 19.758 | -4.191 | 1.00 | 99.22 | A | C |
| ATOM | 917 | O | ASP | 262 | 121.510 | 20.456 | -5.104 | 1.00 | 99.08 | A | O |
| ATOM | 918 | N | ASN | 263 | 121.842 | 19.009 | -3.406 | 1.00 | 48.33 | A | N |
| ATOM | 919 | CA | ASN | 263 | 123.300 | 18.956 | -3.558 | 1.00 | 49.50 | A | C |
| ATOM | 920 | CB | ASN | 263 | 123.896 | 17.820 | -2.719 | 1.00 | 78.20 | A | C |
| ATOM | 921 | CG | ASN | 263 | 123.359 | 17.781 | -1.303 | 1.00 | 82.57 | A | C |
| ATOM | 922 | OD1 | ASN | 263 | 123.578 | 18.703 | -0.511 | 1.00 | 84.07 | A | O |
| ATOM | 923 | ND2 | ASN | 263 | 122.651 | 16.702 | -0.974 | 1.00 | 77.07 | A | N |
| ATOM | 924 | C | ASN | 263 | 123.657 | 18.684 | -5.012 | 1.00 | 50.14 | A | C |
| ATOM | 925 | O | ASN | 263 | 124.574 | 19.286 | -5.572 | 1.00 | 49.04 | A | O |
| ATOM | 926 | N | TYR | 264 | 122.915 | 17.754 | -5.601 | 1.00 | 83.05 | A | N |
| ATOM | 927 | CA | TYR | 264 | 123.112 | 17.330 | -6.976 | 1.00 | 80.90 | A | C |
| ATOM | 928 | CB | TYR | 264 | 121.905 | 16.512 | -7.431 | 1.00 | 165.37 | A | C |
| ATOM | 929 | CG | TYR | 264 | 121.684 | 15.297 | -6.568 | 1.00 | 165.37 | A | C |
| ATOM | 930 | CD1 | TYR | 264 | 121.294 | 15.427 | -5.234 | 1.00 | 165.37 | A | C |
| ATOM | 931 | CE1 | TYR | 264 | 121.137 | 14.312 | -4.419 | 1.00 | 165.37 | A | C |
| ATOM | 932 | CD2 | TYR | 264 | 121.909 | 14.016 | -7.067 | 1.00 | 165.37 | A | C |
| ATOM | 933 | CE2 | TYR | 264 | 121.753 | 12.892 | -6.262 | 1.00 | 165.37 | A | C |
| ATOM | 934 | CZ | TYR | 264 | 121.369 | 13.048 | -4.939 | 1.00 | 165.37 | A | C |
| ATOM | 935 | OH | TYR | 264 | 121.224 | 11.940 | -4.139 | 1.00 | 165.37 | A | O |
| ATOM | 936 | C | TYR | 264 | 123.396 | 18.439 | -7.977 | 1.00 | 79.55 | A | C |
| ATOM | 937 | O | TYR | 264 | 124.509 | 18.536 | -8.498 | 1.00 | 76.68 | A | O |
| ATOM | 938 | N | ARG | 265 | 122.406 | 19.283 | -8.245 | 1.00 | 83.26 | A | N |
| ATOM | 939 | CA | ARG | 265 | 122.605 | 20.340 | -9.224 | 1.00 | 82.16 | A | C |
| ATOM | 940 | CB | ARG | 265 | 121.297 | 20.636 | -9.957 | 1.00 | 36.62 | A | C |
| ATOM | 941 | CG | ARG | 265 | 120.182 | 21.225 | -9.142 | 1.00 | 37.07 | A | C |
| ATOM | 942 | CD | ARG | 265 | 119.267 | 21.953 | -10.110 | 1.00 | 38.90 | A | C |
| ATOM | 943 | NE | ARG | 265 | 118.140 | 22.620 | -9.464 | 1.00 | 44.29 | A | N |
| ATOM | 944 | CZ | ARG | 265 | 117.562 | 23.714 | -9.947 | 1.00 | 44.46 | A | C |
| ATOM | 945 | NH1 | ARG | 265 | 118.016 | 24.257 | -11.071 | 1.00 | 49.09 | A | N |
| ATOM | 946 | NH2 | ARG | 265 | 116.528 | 24.258 | -9.321 | 1.00 | 48.43 | A | N |
| ATOM | 947 | C | ARG | 265 | 123.211 | 21.644 | -8.720 | 1.00 | 81.41 | A | C |
| ATOM | 948 | O | ARG | 265 | 123.137 | 22.668 | -9.396 | 1.00 | 82.72 | A | O |
| ATOM | 949 | N | LEU | 266 | 123.819 | 21.614 | -7.543 | 1.00 | 27.19 | A | N |

# Fig. 19: A-14

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 950 | CA | LEU | 266 | 124.435 | 22.815 | -7.003 | 1.00 | 28.76 | A | C |
| ATOM | 951 | CB | LEU | 266 | 124.798 | 22.601 | -5.539 | 1.00 | 4.24 | A | C |
| ATOM | 952 | CG | LEU | 266 | 125.336 | 23.820 | -4.797 | 1.00 | 3.45 | A | C |
| ATOM | 953 | CD1 | LEU | 266 | 124.393 | 24.999 | -4.976 | 1.00 | 5.79 | A | C |
| ATOM | 954 | CD2 | LEU | 266 | 125.502 | 23.466 | -3.320 | 1.00 | 1.87 | A | C |
| ATOM | 955 | C | LEU | 266 | 125.684 | 23.084 | -7.828 | 1.00 | 31.58 | A | C |
| ATOM | 956 | O | LEU | 266 | 126.086 | 24.226 | -8.022 | 1.00 | 31.46 | A | O |
| ATOM | 957 | N | LYS | 267 | 126.286 | 22.007 | -8.317 | 1.00 | 45.65 | A | N |
| ATOM | 958 | CA | LYS | 267 | 127.479 | 22.088 | -9.149 | 1.00 | 47.96 | A | C |
| ATOM | 959 | CB | LYS | 267 | 127.949 | 20.673 | -9.497 | 1.00 | 72.30 | A | C |
| ATOM | 960 | CG | LYS | 267 | 129.239 | 20.583 | -10.298 | 1.00 | 72.30 | A | C |
| ATOM | 961 | CD | LYS | 267 | 130.428 | 20.277 | -9.403 | 1.00 | 72.30 | A | C |
| ATOM | 962 | CE | LYS | 267 | 131.649 | 19.894 | -10.230 | 1.00 | 72.30 | A | C |
| ATOM | 963 | NZ | LYS | 267 | 132.793 | 19.452 | -9.381 | 1.00 | 72.30 | A | N |
| ATOM | 964 | C | LYS | 267 | 127.103 | 22.842 | -10.427 | 1.00 | 47.45 | A | C |
| ATOM | 965 | O | LYS | 267 | 127.763 | 23.810 | -10.809 | 1.00 | 46.97 | A | O |
| ATOM | 966 | N | GLN | 268 | 126.032 | 22.389 | -11.074 | 1.00 | 32.65 | A | N |
| ATOM | 967 | CA | GLN | 268 | 125.553 | 22.999 | -12.303 | 1.00 | 31.62 | A | C |
| ATOM | 968 | CB | GLN | 268 | 124.292 | 22.295 | -12.798 | 1.00 | 88.56 | A | C |
| ATOM | 969 | CG | GLN | 268 | 124.449 | 20.845 | -13.182 | 1.00 | 88.56 | A | C |
| ATOM | 970 | CD | GLN | 268 | 123.119 | 20.227 | -13.576 | 1.00 | 88.56 | A | C |
| ATOM | 971 | OE1 | GLN | 268 | 123.059 | 19.078 | -14.010 | 1.00 | 88.56 | A | O |
| ATOM | 972 | NE2 | GLN | 268 | 122.041 | 20.992 | -13.423 | 1.00 | 88.56 | A | N |
| ATOM | 973 | C | GLN | 268 | 125.221 | 24.474 | -12.100 | 1.00 | 27.37 | A | C |
| ATOM | 974 | O | GLN | 268 | 125.678 | 25.332 | -12.851 | 1.00 | 28.55 | A | O |
| ATOM | 975 | N | VAL | 269 | 124.410 | 24.767 | -11.089 | 1.00 | 11.19 | A | N |
| ATOM | 976 | CA | VAL | 269 | 124.007 | 26.140 | -10.830 | 1.00 | 8.94 | A | C |
| ATOM | 977 | CB | VAL | 269 | 123.088 | 26.223 | -9.598 | 1.00 | 22.95 | A | C |
| ATOM | 978 | CG1 | VAL | 269 | 122.650 | 27.667 | -9.374 | 1.00 | 18.60 | A | C |
| ATOM | 979 | CG2 | VAL | 269 | 121.872 | 25.334 | -9.801 | 1.00 | 20.81 | A | C |
| ATOM | 980 | C | VAL | 269 | 125.198 | 27.076 | -10.649 | 1.00 | 8.53 | A | C |
| ATOM | 981 | O | VAL | 269 | 125.286 | 28.093 | -11.318 | 1.00 | 11.37 | A | O |
| ATOM | 982 | N | ILE | 270 | 126.114 | 26.744 | -9.746 | 1.00 | 5.57 | A | N |
| ATOM | 983 | CA | ILE | 270 | 127.291 | 27.585 | -9.535 | 1.00 | 6.19 | A | C |
| ATOM | 984 | CB | ILE | 270 | 128.281 | 26.944 | -8.533 | 1.00 | 12.81 | A | C |
| ATOM | 985 | CG2 | ILE | 270 | 129.592 | 27.731 | -8.504 | 1.00 | 7.43 | A | C |
| ATOM | 986 | CG1 | ILE | 270 | 127.671 | 26.926 | -7.135 | 1.00 | 10.37 | A | C |
| ATOM | 987 | CD1 | ILE | 270 | 127.367 | 28.317 | -6.591 | 1.00 | 11.49 | A | C |
| ATOM | 988 | C | ILE | 270 | 128.001 | 27.775 | -10.870 | 1.00 | 10.06 | A | C |
| ATOM | 989 | O | ILE | 270 | 128.549 | 28.838 | -11.140 | 1.00 | 8.84 | A | O |
| ATOM | 990 | N | GLN | 271 | 127.981 | 26.729 | -11.696 | 1.00 | 7.96 | A | N |
| ATOM | 991 | CA | GLN | 271 | 128.605 | 26.751 | -13.011 | 1.00 | 10.02 | A | C |
| ATOM | 992 | CB | GLN | 271 | 128.434 | 25.394 | -13.698 | 1.00 | 84.89 | A | C |
| ATOM | 993 | CG | GLN | 271 | 129.267 | 25.214 | -14.947 | 1.00 | 86.79 | A | C |
| ATOM | 994 | CD | GLN | 271 | 130.744 | 25.366 | -14.665 | 1.00 | 89.29 | A | C |
| ATOM | 995 | OE1 | GLN | 271 | 131.244 | 26.477 | -14.506 | 1.00 | 89.62 | A | O |
| ATOM | 996 | NE2 | GLN | 271 | 131.451 | 24.243 | -14.583 | 1.00 | 90.86 | A | N |
| ATOM | 997 | C | GLN | 271 | 127.962 | 27.842 | -13.860 | 1.00 | 12.48 | A | C |
| ATOM | 998 | O | GLN | 271 | 128.644 | 28.733 | -14.348 | 1.00 | 15.17 | A | O |
| ATOM | 999 | N | ASP | 272 | 126.648 | 27.770 | -14.031 | 1.00 | 33.57 | A | N |
| ATOM | 1000 | CA | ASP | 272 | 125.929 | 28.758 | -14.818 | 1.00 | 34.85 | A | C |
| ATOM | 1001 | CB | ASP | 272 | 124.430 | 28.459 | -14.786 | 1.00 | 74.39 | A | C |
| ATOM | 1002 | CG | ASP | 272 | 124.084 | 27.142 | -15.454 | 1.00 | 76.01 | A | C |
| ATOM | 1003 | OD1 | ASP | 272 | 123.000 | 26.589 | -15.163 | 1.00 | 78.08 | A | O |
| ATOM | 1004 | OD2 | ASP | 272 | 124.893 | 26.665 | -16.278 | 1.00 | 82.27 | A | O |
| ATOM | 1005 | C | ASP | 272 | 126.194 | 30.163 | -14.283 | 1.00 | 35.65 | A | C |
| ATOM | 1006 | O | ASP | 272 | 126.190 | 31.131 | -15.042 | 1.00 | 33.10 | A | O |
| ATOM | 1007 | N | CYS | 273 | 126.426 | 30.280 | -12.978 | 1.00 | 42.88 | A | N |
| ATOM | 1008 | CA | CYS | 273 | 126.698 | 31.582 | -12.387 | 1.00 | 41.31 | A | C |
| ATOM | 1009 | CB | CYS | 273 | 126.630 | 31.516 | -10.862 | 1.00 | 24.14 | A | C |
| ATOM | 1010 | SG | CYS | 273 | 124.940 | 31.489 | -10.191 | 1.00 | 22.24 | A | S |
| ATOM | 1011 | C | CYS | 273 | 128.059 | 32.090 | -12.826 | 1.00 | 41.68 | A | C |
| ATOM | 1012 | O | CYS | 273 | 128.244 | 33.288 | -13.008 | 1.00 | 35.99 | A | O |
| ATOM | 1013 | N | GLU | 274 | 129.010 | 31.178 | -12.994 | 1.00 | 20.07 | A | N |
| ATOM | 1014 | CA | GLU | 274 | 130.364 | 31.531 | -13.440 | 1.00 | 22.87 | A | C |
| ATOM | 1015 | CB | GLU | 274 | 131.317 | 30.338 | -13.298 | 1.00 | 39.18 | A | C |
| ATOM | 1016 | CG | GLU | 274 | 132.090 | 30.309 | -11.989 | 1.00 | 44.30 | A | C |
| ATOM | 1017 | CD | GLU | 274 | 133.041 | 31.490 | -11.836 | 1.00 | 49.41 | A | C |
| ATOM | 1018 | OE1 | GLU | 274 | 133.622 | 31.659 | -10.740 | 1.00 | 51.28 | A | O |
| ATOM | 1019 | OE2 | GLU | 274 | 133.212 | 32.251 | -12.812 | 1.00 | 53.97 | A | O |
| ATOM | 1020 | C | GLU | 274 | 130.345 | 31.984 | -14.893 | 1.00 | 25.29 | A | C |
| ATOM | 1021 | O | GLU | 274 | 131.031 | 32.931 | -15.266 | 1.00 | 27.49 | A | O |
| ATOM | 1022 | N | ASP | 275 | 129.550 | 31.298 | -15.707 | 1.00 | 41.03 | A | N |

Fig. 19: A-15

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1023 | CA | ASP | 275 | 129.421 | 31.625 | -17.119 | 1.00 | 39.77 | A | C |
| ATOM | 1024 | CB | ASP | 275 | 128.538 | 30.594 | -17.822 | 1.00 | 63.42 | A | C |
| ATOM | 1025 | CG | ASP | 275 | 129.106 | 29.203 | -17.757 | 1.00 | 64.69 | A | C |
| ATOM | 1026 | OD1 | ASP | 275 | 129.987 | 28.959 | -16.906 | 1.00 | 68.39 | A | O |
| ATOM | 1027 | OD2 | ASP | 275 | 128.657 | 28.352 | -18.551 | 1.00 | 66.35 | A | O |
| ATOM | 1028 | C | ASP | 275 | 128.789 | 32.996 | -17.295 | 1.00 | 38.76 | A | C |
| ATOM | 1029 | O | ASP | 275 | 128.883 | 33.595 | -18.367 | 1.00 | 34.31 | A | O |
| ATOM | 1030 | N | GLU | 276 | 128.137 | 33.485 | -16.247 | 1.00 | 28.36 | A | N |
| ATOM | 1031 | CA | GLU | 276 | 127.479 | 34.771 | -16.328 | 1.00 | 28.01 | A | C |
| ATOM | 1032 | CB | GLU | 276 | 126.019 | 34.617 | -15.913 | 1.00 | 53.33 | A | C |
| ATOM | 1033 | CG | GLU | 276 | 125.310 | 33.520 | -16.700 | 1.00 | 53.20 | A | C |
| ATOM | 1034 | CD | GLU | 276 | 123.807 | 33.493 | -16.487 | 1.00 | 54.30 | A | C |
| ATOM | 1035 | OE1 | GLU | 276 | 123.150 | 32.629 | -17.102 | 1.00 | 55.01 | A | O |
| ATOM | 1036 | OE2 | GLU | 276 | 123.280 | 34.330 | -15.717 | 1.00 | 51.24 | A | O |
| ATOM | 1037 | C | GLU | 276 | 128.172 | 35.841 | -15.504 | 1.00 | 26.84 | A | C |
| ATOM | 1038 | O | GLU | 276 | 127.621 | 36.919 | -15.288 | 1.00 | 27.95 | A | O |
| ATOM | 1039 | N | ASN | 277 | 129.382 | 35.535 | -15.050 | 1.00 | 28.50 | A | N |
| ATOM | 1040 | CA | ASN | 277 | 130.185 | 36.472 | -14.268 | 1.00 | 28.47 | A | C |
| ATOM | 1041 | CB | ASN | 277 | 130.607 | 37.655 | -15.140 | 1.00 | 86.35 | A | C |
| ATOM | 1042 | CG | ASN | 277 | 131.230 | 37.218 | -16.439 | 1.00 | 91.27 | A | C |
| ATOM | 1043 | OD1 | ASN | 277 | 132.263 | 36.548 | -16.451 | 1.00 | 91.09 | A | O |
| ATOM | 1044 | ND2 | ASN | 277 | 130.601 | 37.589 | -17.550 | 1.00 | 90.23 | A | N |
| ATOM | 1045 | C | ASN | 277 | 129.493 | 37.014 | -13.018 | 1.00 | 24.82 | A | C |
| ATOM | 1046 | O | ASN | 277 | 129.476 | 38.226 | -12.790 | 1.00 | 25.80 | A | O |
| ATOM | 1047 | N | ILE | 278 | 128.925 | 36.127 | -12.207 | 1.00 | 15.37 | A | N |
| ATOM | 1048 | CA | ILE | 278 | 128.261 | 36.560 | -10.989 | 1.00 | 15.82 | A | C |
| ATOM | 1049 | CB | ILE | 278 | 126.963 | 35.773 | -10.747 | 1.00 | 17.43 | A | C |
| ATOM | 1050 | CG2 | ILE | 278 | 126.304 | 36.243 | -9.454 | 1.00 | 18.82 | A | C |
| ATOM | 1051 | CG1 | ILE | 278 | 126.016 | 35.949 | -11.932 | 1.00 | 14.88 | A | C |
| ATOM | 1052 | CD1 | ILE | 278 | 124.742 | 35.153 | -11.796 | 1.00 | 17.16 | A | C |
| ATOM | 1053 | C | ILE | 278 | 129.168 | 36.345 | -9.780 | 1.00 | 16.42 | A | C |
| ATOM | 1054 | O | ILE | 278 | 129.363 | 35.212 | -9.354 | 1.00 | 16.76 | A | O |
| ATOM | 1055 | N | GLN | 279 | 129.737 | 37.426 | -9.244 | 1.00 | 26.25 | A | N |
| ATOM | 1056 | CA | GLN | 279 | 130.578 | 37.335 | -8.053 | 1.00 | 25.85 | A | C |
| ATOM | 1057 | CB | GLN | 279 | 131.035 | 38.716 | -7.605 | 1.00 | 41.76 | A | C |
| ATOM | 1058 | CG | GLN | 279 | 131.959 | 39.382 | -8.574 | 1.00 | 47.54 | A | C |
| ATOM | 1059 | CD | GLN | 279 | 133.158 | 38.524 | -8.894 | 1.00 | 51.46 | A | C |
| ATOM | 1060 | OE1 | GLN | 279 | 133.992 | 38.255 | -8.023 | 1.00 | 45.70 | A | O |
| ATOM | 1061 | NE2 | GLN | 279 | 133.252 | 38.078 | -10.146 | 1.00 | 51.05 | A | N |
| ATOM | 1062 | C | GLN | 279 | 129.716 | 36.736 | -6.958 | 1.00 | 23.72 | A | C |
| ATOM | 1063 | O | GLN | 279 | 128.609 | 37.216 | -6.692 | 1.00 | 20.64 | A | O |
| ATOM | 1064 | N | ARG | 280 | 130.214 | 35.697 | -6.310 | 1.00 | 16.06 | A | N |
| ATOM | 1065 | CA | ARG | 280 | 129.440 | 35.054 | -5.258 | 1.00 | 17.58 | A | C |
| ATOM | 1066 | CB | ARG | 280 | 129.107 | 33.620 | -5.661 | 1.00 | 19.51 | A | C |
| ATOM | 1067 | CG | ARG | 280 | 128.413 | 33.488 | -6.997 | 1.00 | 18.14 | A | C |
| ATOM | 1068 | CD | ARG | 280 | 128.274 | 32.021 | -7.371 | 1.00 | 17.81 | A | C |
| ATOM | 1069 | NE | ARG | 280 | 129.576 | 31.365 | -7.441 | 1.00 | 14.86 | A | N |
| ATOM | 1070 | CZ | ARG | 280 | 130.427 | 31.489 | -8.452 | 1.00 | 18.77 | A | C |
| ATOM | 1071 | NH1 | ARG | 280 | 130.131 | 32.241 | -9.493 | 1.00 | 21.69 | A | N |
| ATOM | 1072 | NH2 | ARG | 280 | 131.579 | 30.846 | -8.422 | 1.00 | 23.71 | A | N |
| ATOM | 1073 | C | ARG | 280 | 130.123 | 35.037 | -3.892 | 1.00 | 17.24 | A | C |
| ATOM | 1074 | O | ARG | 280 | 131.269 | 34.592 | -3.750 | 1.00 | 16.97 | A | O |
| ATOM | 1075 | N | PHE | 281 | 129.406 | 35.539 | -2.894 | 1.00 | 21.33 | A | N |
| ATOM | 1076 | CA | PHE | 281 | 129.889 | 35.538 | -1.527 | 1.00 | 23.32 | A | C |
| ATOM | 1077 | CB | PHE | 281 | 129.848 | 36.933 | -0.924 | 1.00 | 12.67 | A | C |
| ATOM | 1078 | CG | PHE | 281 | 130.754 | 37.900 | -1.603 | 1.00 | 15.70 | A | C |
| ATOM | 1079 | CD1 | PHE | 281 | 130.419 | 38.434 | -2.837 | 1.00 | 19.55 | A | C |
| ATOM | 1080 | CD2 | PHE | 281 | 131.968 | 38.250 | -1.024 | 1.00 | 17.43 | A | C |
| ATOM | 1081 | CE1 | PHE | 281 | 131.281 | 39.305 | -3.487 | 1.00 | 19.61 | A | C |
| ATOM | 1082 | CE2 | PHE | 281 | 132.842 | 39.120 | -1.665 | 1.00 | 15.16 | A | C |
| ATOM | 1083 | CZ | PHE | 281 | 132.498 | 39.650 | -2.900 | 1.00 | 16.59 | A | C |
| ATOM | 1084 | C | PHE | 281 | 128.925 | 34.646 | -0.785 | 1.00 | 24.03 | A | C |
| ATOM | 1085 | O | PHE | 281 | 127.710 | 34.867 | -0.821 | 1.00 | 26.40 | A | O |
| ATOM | 1086 | N | SER | 282 | 129.449 | 33.613 | -0.141 | 1.00 | 13.47 | A | N |
| ATOM | 1087 | CA | SER | 282 | 128.594 | 32.705 | 0.602 | 1.00 | 15.32 | A | C |
| ATOM | 1088 | CB | SER | 282 | 128.746 | 31.272 | 0.084 | 1.00 | 11.38 | A | C |
| ATOM | 1089 | OG | SER | 282 | 130.081 | 30.816 | 0.216 | 1.00 | 7.93 | A | O |
| ATOM | 1090 | C | SER | 282 | 128.947 | 32.782 | 2.069 | 1.00 | 17.20 | A | C |
| ATOM | 1091 | O | SER | 282 | 130.066 | 33.135 | 2.435 | 1.00 | 21.06 | A | O |
| ATOM | 1092 | N | ILE | 283 | 127.969 | 32.477 | 2.908 | 1.00 | 24.08 | A | N |
| ATOM | 1093 | CA | ILE | 283 | 128.164 | 32.504 | 4.343 | 1.00 | 22.00 | A | C |
| ATOM | 1094 | CB | ILE | 283 | 127.517 | 33.733 | 4.968 | 1.00 | 17.91 | A | C |
| ATOM | 1095 | CG2 | ILE | 283 | 127.843 | 33.791 | 6.442 | 1.00 | 18.72 | A | C |

# Fig. 19: A-16

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1096 | CG1 | ILE | 283 | 128.045 | 34.986 | 4.281 | 1.00 | 14.38 | A | C |
| ATOM | 1097 | CD1 | ILE | 283 | 127.103 | 36.171 | 4.383 | 1.00 | 17.94 | A | C |
| ATOM | 1098 | C | ILE | 283 | 127.510 | 31.273 | 4.912 | 1.00 | 21.07 | A | C |
| ATOM | 1099 | O | ILE | 283 | 126.394 | 30.917 | 4.536 | 1.00 | 20.93 | A | O |
| ATOM | 1100 | N | ALA | 284 | 128.204 | 30.618 | 5.823 | 1.00 | 29.93 | A | N |
| ATOM | 1101 | CA | ALA | 284 | 127.663 | 29.421 | 6.412 | 1.00 | 29.95 | A | C |
| ATOM | 1102 | CB | ALA | 284 | 128.548 | 28.253 | 6.070 | 1.00 | 1.87 | A | C |
| ATOM | 1103 | C | ALA | 284 | 127.507 | 29.536 | 7.920 | 1.00 | 28.08 | A | C |
| ATOM | 1104 | O | ALA | 284 | 128.482 | 29.740 | 8.641 | 1.00 | 26.74 | A | O |
| ATOM | 1105 | N | ILE | 285 | 126.270 | 29.422 | 8.389 | 1.00 | 31.23 | A | N |
| ATOM | 1106 | CA | ILE | 285 | 125.997 | 29.457 | 9.817 | 1.00 | 25.43 | A | C |
| ATOM | 1107 | CB | ILE | 285 | 124.529 | 29.859 | 10.107 | 1.00 | 43.54 | A | C |
| ATOM | 1108 | CG2 | ILE | 285 | 124.187 | 29.569 | 11.555 | 1.00 | 38.36 | A | C |
| ATOM | 1109 | CG1 | ILE | 285 | 124.306 | 31.344 | 9.791 | 1.00 | 38.87 | A | C |
| ATOM | 1110 | CD1 | ILE | 285 | 124.206 | 31.670 | 8.315 | 1.00 | 40.01 | A | C |
| ATOM | 1111 | C | ILE | 285 | 126.227 | 28.022 | 10.296 | 1.00 | 28.75 | A | C |
| ATOM | 1112 | O | ILE | 285 | 125.523 | 27.106 | 9.872 | 1.00 | 30.49 | A | O |
| ATOM | 1113 | N | LEU | 286 | 127.205 | 27.818 | 11.169 | 1.00 | 38.23 | A | N |
| ATOM | 1114 | CA | LEU | 286 | 127.497 | 26.471 | 11.649 | 1.00 | 38.71 | A | C |
| ATOM | 1115 | CB | LEU | 286 | 128.999 | 26.313 | 11.876 | 1.00 | 50.51 | A | C |
| ATOM | 1116 | CG | LEU | 286 | 129.917 | 26.722 | 10.727 | 1.00 | 53.33 | A | C |
| ATOM | 1117 | CD1 | LEU | 286 | 131.340 | 26.363 | 11.105 | 1.00 | 55.89 | A | C |
| ATOM | 1118 | CD2 | LEU | 286 | 129.513 | 26.019 | 9.441 | 1.00 | 55.00 | A | C |
| ATOM | 1119 | C | LEU | 286 | 126.760 | 26.069 | 12.923 | 1.00 | 39.16 | A | C |
| ATOM | 1120 | O | LEU | 286 | 127.068 | 25.036 | 13.517 | 1.00 | 40.00 | A | O |
| ATOM | 1121 | N | GLY | 287 | 125.789 | 26.875 | 13.339 | 1.00 | 72.80 | A | N |
| ATOM | 1122 | CA | GLY | 287 | 125.042 | 26.579 | 14.551 | 1.00 | 71.58 | A | C |
| ATOM | 1123 | C | GLY | 287 | 124.586 | 25.139 | 14.700 | 1.00 | 69.16 | A | C |
| ATOM | 1124 | O | GLY | 287 | 125.056 | 24.419 | 15.583 | 1.00 | 73.26 | A | O |
| ATOM | 1125 | N | THR | 296 | 131.112 | 19.210 | 10.542 | 1.00 | 87.02 | A | N |
| ATOM | 1126 | CA | THR | 296 | 130.609 | 20.333 | 9.766 | 1.00 | 87.06 | A | C |
| ATOM | 1127 | CB | THR | 296 | 130.702 | 21.652 | 10.554 | 1.00 | 100.17 | A | C |
| ATOM | 1128 | OG1 | THR | 296 | 132.071 | 21.903 | 10.895 | 1.00 | 105.23 | A | O |
| ATOM | 1129 | CG2 | THR | 296 | 129.861 | 21.592 | 11.817 | 1.00 | 100.04 | A | C |
| ATOM | 1130 | C | THR | 296 | 131.387 | 20.535 | 8.479 | 1.00 | 88.04 | A | C |
| ATOM | 1131 | O | THR | 296 | 130.985 | 21.331 | 7.631 | 1.00 | 86.85 | A | O |
| ATOM | 1132 | N | GLU | 297 | 132.497 | 19.825 | 8.322 | 1.00 | 78.34 | A | N |
| ATOM | 1133 | CA | GLU | 297 | 133.304 | 20.020 | 7.128 | 1.00 | 81.80 | A | C |
| ATOM | 1134 | CB | GLU | 297 | 134.577 | 19.171 | 7.169 | 1.00 | 125.47 | A | C |
| ATOM | 1135 | CG | GLU | 297 | 134.403 | 17.709 | 6.851 | 1.00 | 132.50 | A | C |
| ATOM | 1136 | CD | GLU | 297 | 135.690 | 17.103 | 6.342 | 1.00 | 133.75 | A | C |
| ATOM | 1137 | OE1 | GLU | 297 | 135.709 | 15.886 | 6.067 | 1.00 | 135.24 | A | O |
| ATOM | 1138 | OE2 | GLU | 297 | 136.682 | 17.853 | 6.212 | 1.00 | 137.19 | A | O |
| ATOM | 1139 | C | GLU | 297 | 132.550 | 19.770 | 5.832 | 1.00 | 79.84 | A | C |
| ATOM | 1140 | O | GLU | 297 | 132.581 | 20.609 | 4.931 | 1.00 | 79.34 | A | O |
| ATOM | 1141 | N | LYS | 298 | 131.865 | 18.638 | 5.728 | 1.00 | 42.69 | A | N |
| ATOM | 1142 | CA | LYS | 298 | 131.125 | 18.352 | 4.505 | 1.00 | 42.69 | A | C |
| ATOM | 1143 | CB | LYS | 298 | 130.281 | 17.087 | 4.678 | 1.00 | 102.63 | A | C |
| ATOM | 1144 | CG | LYS | 298 | 129.695 | 16.562 | 3.376 | 1.00 | 111.34 | A | C |
| ATOM | 1145 | CD | LYS | 298 | 129.117 | 15.166 | 3.545 | 1.00 | 113.06 | A | C |
| ATOM | 1146 | CE | LYS | 298 | 130.167 | 14.187 | 4.057 | 1.00 | 116.88 | A | C |
| ATOM | 1147 | NZ | LYS | 298 | 131.378 | 14.159 | 3.195 | 1.00 | 121.20 | A | N |
| ATOM | 1148 | C | LYS | 298 | 130.228 | 19.547 | 4.143 | 1.00 | 40.29 | A | C |
| ATOM | 1149 | O | LYS | 298 | 130.032 | 19.853 | 2.964 | 1.00 | 41.17 | A | O |
| ATOM | 1150 | N | PHE | 299 | 129.700 | 20.218 | 5.167 | 1.00 | 38.43 | A | N |
| ATOM | 1151 | CA | PHE | 299 | 128.839 | 21.380 | 4.978 | 1.00 | 36.67 | A | C |
| ATOM | 1152 | CB | PHE | 299 | 128.100 | 21.712 | 6.283 | 1.00 | 55.97 | A | C |
| ATOM | 1153 | CG | PHE | 299 | 127.256 | 22.967 | 6.209 | 1.00 | 48.41 | A | C |
| ATOM | 1154 | CD1 | PHE | 299 | 126.319 | 23.146 | 5.186 | 1.00 | 44.86 | A | C |
| ATOM | 1155 | CD2 | PHE | 299 | 127.400 | 23.970 | 7.160 | 1.00 | 46.14 | A | C |
| ATOM | 1156 | CE1 | PHE | 299 | 125.545 | 24.307 | 5.117 | 1.00 | 44.27 | A | C |
| ATOM | 1157 | CE2 | PHE | 299 | 126.627 | 25.132 | 7.095 | 1.00 | 40.55 | A | C |
| ATOM | 1158 | CZ | PHE | 299 | 125.701 | 25.299 | 6.073 | 1.00 | 39.06 | A | C |
| ATOM | 1159 | C | PHE | 299 | 129.684 | 22.573 | 4.544 | 1.00 | 37.02 | A | C |
| ATOM | 1160 | O | PHE | 299 | 129.439 | 23.190 | 3.504 | 1.00 | 32.83 | A | O |
| ATOM | 1161 | N | VAL | 300 | 130.682 | 22.896 | 5.352 | 1.00 | 13.94 | A | N |
| ATOM | 1162 | CA | VAL | 300 | 131.551 | 24.010 | 5.034 | 1.00 | 18.89 | A | C |
| ATOM | 1163 | CB | VAL | 300 | 132.752 | 24.068 | 5.993 | 1.00 | 40.51 | A | C |
| ATOM | 1164 | CG1 | VAL | 300 | 133.769 | 25.076 | 5.493 | 1.00 | 44.08 | A | C |
| ATOM | 1165 | CG2 | VAL | 300 | 132.282 | 24.451 | 7.382 | 1.00 | 44.52 | A | C |
| ATOM | 1166 | C | VAL | 300 | 132.061 | 23.893 | 3.607 | 1.00 | 17.53 | A | C |
| ATOM | 1167 | O | VAL | 300 | 132.177 | 24.889 | 2.906 | 1.00 | 18.03 | A | O |
| ATOM | 1168 | N | GLU | 301 | 132.365 | 22.679 | 3.164 | 1.00 | 18.30 | A | N |

Fig. 19: A-17

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1169 | CA | GLU | 301 | 132.866 | 22.513 | 1.808 | 1.00 | 18.96 | A | C |
| ATOM | 1170 | CB | GLU | 301 | 133.407 | 21.094 | 1.605 | 1.00 | 40.16 | A | C |
| ATOM | 1171 | CG | GLU | 301 | 134.058 | 20.854 | 0.243 | 1.00 | 42.43 | A | C |
| ATOM | 1172 | CD | GLU | 301 | 135.049 | 21.943 | -0.155 | 1.00 | 48.24 | A | C |
| ATOM | 1173 | OE1 | GLU | 301 | 135.956 | 22.267 | 0.645 | 1.00 | 47.79 | A | O |
| ATOM | 1174 | OE2 | GLU | 301 | 134.918 | 22.469 | -1.282 | 1.00 | 50.51 | A | O |
| ATOM | 1175 | C | GLU | 301 | 131.770 | 22.832 | 0.791 | 1.00 | 17.53 | A | C |
| ATOM | 1176 | O | GLU | 301 | 132.034 | 23.458 | -0.242 | 1.00 | 15.61 | A | O |
| ATOM | 1177 | N | GLU | 302 | 130.541 | 22.420 | 1.097 | 1.00 | 32.12 | A | N |
| ATOM | 1178 | CA | GLU | 302 | 129.412 | 22.667 | 0.210 | 1.00 | 31.93 | A | C |
| ATOM | 1179 | CB | GLU | 302 | 128.127 | 22.084 | 0.801 | 1.00 | 76.04 | A | C |
| ATOM | 1180 | CG | GLU | 302 | 126.894 | 22.274 | -0.071 | 1.00 | 75.79 | A | C |
| ATOM | 1181 | CD | GLU | 302 | 125.659 | 21.594 | 0.501 | 1.00 | 72.72 | A | C |
| ATOM | 1182 | OE1 | GLU | 302 | 125.651 | 20.349 | 0.584 | 1.00 | 72.70 | A | O |
| ATOM | 1183 | OE2 | GLU | 302 | 124.698 | 22.302 | 0.872 | 1.00 | 77.14 | A | O |
| ATOM | 1184 | C | GLU | 302 | 129.237 | 24.158 | -0.033 | 1.00 | 35.00 | A | C |
| ATOM | 1185 | O | GLU | 302 | 129.040 | 24.580 | -1.170 | 1.00 | 34.26 | A | O |
| ATOM | 1186 | N | ILE | 303 | 129.334 | 24.953 | 1.031 | 1.00 | 23.69 | A | N |
| ATOM | 1187 | CA | ILE | 303 | 129.171 | 26.405 | 0.936 | 1.00 | 23.74 | A | C |
| ATOM | 1188 | CB | ILE | 303 | 128.933 | 27.019 | 2.326 | 1.00 | 28.42 | A | C |
| ATOM | 1189 | CG2 | ILE | 303 | 128.556 | 28.480 | 2.199 | 1.00 | 23.60 | A | C |
| ATOM | 1190 | CG1 | ILE | 303 | 127.823 | 26.245 | 3.046 | 1.00 | 26.02 | A | C |
| ATOM | 1191 | CD1 | ILE | 303 | 126.599 | 25.926 | 2.183 | 1.00 | 22.48 | A | C |
| ATOM | 1192 | C | ILE | 303 | 130.340 | 27.129 | 0.267 | 1.00 | 25.77 | A | C |
| ATOM | 1193 | O | ILE | 303 | 130.133 | 28.036 | -0.553 | 1.00 | 28.26 | A | O |
| ATOM | 1194 | N | LYS | 304 | 131.564 | 26.740 | 0.612 | 1.00 | 28.18 | A | N |
| ATOM | 1195 | CA | LYS | 304 | 132.733 | 27.363 | 0.003 | 1.00 | 28.98 | A | C |
| ATOM | 1196 | CB | LYS | 304 | 134.018 | 26.713 | 0.501 | 1.00 | 31.11 | A | C |
| ATOM | 1197 | CG | LYS | 304 | 134.415 | 27.051 | 1.915 | 1.00 | 37.78 | A | C |
| ATOM | 1198 | CD | LYS | 304 | 135.810 | 26.502 | 2.190 | 1.00 | 39.31 | A | C |
| ATOM | 1199 | CE | LYS | 304 | 136.298 | 26.803 | 3.599 | 1.00 | 42.04 | A | C |
| ATOM | 1200 | NZ | LYS | 304 | 137.673 | 26.262 | 3.857 | 1.00 | 44.22 | A | N |
| ATOM | 1201 | C | LYS | 304 | 132.665 | 27.210 | -1.512 | 1.00 | 25.07 | A | C |
| ATOM | 1202 | O | LYS | 304 | 133.033 | 28.118 | -2.252 | 1.00 | 29.15 | A | O |
| ATOM | 1203 | N | SER | 305 | 132.195 | 26.054 | -1.965 | 1.00 | 30.32 | A | N |
| ATOM | 1204 | CA | SER | 305 | 132.100 | 25.785 | -3.386 | 1.00 | 27.48 | A | C |
| ATOM | 1205 | CB | SER | 305 | 131.702 | 24.329 | -3.635 | 1.00 | 18.09 | A | C |
| ATOM | 1206 | OG | SER | 305 | 130.352 | 24.088 | -3.293 | 1.00 | 14.77 | A | O |
| ATOM | 1207 | C | SER | 305 | 131.094 | 26.709 | -4.044 | 1.00 | 28.00 | A | C |
| ATOM | 1208 | O | SER | 305 | 131.137 | 26.917 | -5.263 | 1.00 | 30.57 | A | O |
| ATOM | 1209 | N | ILE | 306 | 130.181 | 27.258 | -3.247 | 1.00 | 37.08 | A | N |
| ATOM | 1210 | CA | ILE | 306 | 129.180 | 28.176 | -3.783 | 1.00 | 33.83 | A | C |
| ATOM | 1211 | CB | ILE | 306 | 127.990 | 28.319 | -2.831 | 1.00 | 15.00 | A | C |
| ATOM | 1212 | CG2 | ILE | 306 | 127.190 | 29.565 | -3.167 | 1.00 | 15.73 | A | C |
| ATOM | 1213 | CG1 | ILE | 306 | 127.118 | 27.069 | -2.929 | 1.00 | 17.63 | A | C |
| ATOM | 1214 | CD1 | ILE | 306 | 125.993 | 27.029 | -1.916 | 1.00 | 15.34 | A | C |
| ATOM | 1215 | C | ILE | 306 | 129.812 | 29.544 | -4.008 | 1.00 | 31.59 | A | C |
| ATOM | 1216 | O | ILE | 306 | 129.361 | 30.333 | -4.851 | 1.00 | 32.12 | A | O |
| ATOM | 1217 | N | ALA | 307 | 130.874 | 29.805 | -3.251 | 1.00 | 20.26 | A | N |
| ATOM | 1218 | CA | ALA | 307 | 131.584 | 31.062 | -3.349 | 1.00 | 22.45 | A | C |
| ATOM | 1219 | CB | ALA | 307 | 132.444 | 31.260 | -2.118 | 1.00 | 5.65 | A | C |
| ATOM | 1220 | C | ALA | 307 | 132.441 | 31.113 | -4.611 | 1.00 | 22.11 | A | C |
| ATOM | 1221 | O | ALA | 307 | 132.622 | 30.103 | -5.302 | 1.00 | 21.10 | A | O |
| ATOM | 1222 | N | SER | 308 | 132.953 | 32.307 | -4.906 | 1.00 | 24.29 | A | N |
| ATOM | 1223 | CA | SER | 308 | 133.796 | 32.533 | -6.072 | 1.00 | 27.22 | A | C |
| ATOM | 1224 | CB | SER | 308 | 133.489 | 33.899 | -6.700 | 1.00 | 15.61 | A | C |
| ATOM | 1225 | OG | SER | 308 | 132.299 | 33.860 | -7.460 | 1.00 | 19.00 | A | O |
| ATOM | 1226 | C | SER | 308 | 135.264 | 32.482 | -5.690 | 1.00 | 30.87 | A | C |
| ATOM | 1227 | O | SER | 308 | 135.625 | 32.797 | -4.555 | 1.00 | 28.21 | A | O |
| ATOM | 1228 | N | GLU | 309 | 136.103 | 32.069 | -6.640 | 1.00 | 26.43 | A | N |
| ATOM | 1229 | CA | GLU | 309 | 137.542 | 32.008 | -6.418 | 1.00 | 29.92 | A | C |
| ATOM | 1230 | CB | GLU | 309 | 138.224 | 31.266 | -7.569 | 1.00 | 73.14 | A | C |
| ATOM | 1231 | CG | GLU | 309 | 137.811 | 29.809 | -7.737 | 1.00 | 78.51 | A | C |
| ATOM | 1232 | CD | GLU | 309 | 138.181 | 28.950 | -6.541 | 1.00 | 81.27 | A | C |
| ATOM | 1233 | OE1 | GLU | 309 | 138.103 | 27.708 | -6.651 | 1.00 | 83.60 | A | O |
| ATOM | 1234 | OE2 | GLU | 309 | 138.544 | 29.514 | -5.487 | 1.00 | 85.42 | A | O |
| ATOM | 1235 | C | GLU | 309 | 138.009 | 33.461 | -6.396 | 1.00 | 30.67 | A | C |
| ATOM | 1236 | O | GLU | 309 | 137.580 | 34.257 | -7.230 | 1.00 | 32.32 | A | O |
| ATOM | 1237 | N | PRO | 310 | 138.882 | 33.834 | -5.442 | 1.00 | 19.51 | A | N |
| ATOM | 1238 | CD | PRO | 310 | 139.395 | 35.217 | -5.381 | 1.00 | 49.07 | A | C |
| ATOM | 1239 | CA | PRO | 310 | 139.483 | 33.029 | -4.377 | 1.00 | 19.70 | A | C |
| ATOM | 1240 | CB | PRO | 310 | 140.703 | 33.851 | -3.982 | 1.00 | 50.90 | A | C |
| ATOM | 1241 | CG | PRO | 310 | 140.182 | 35.231 | -4.065 | 1.00 | 50.46 | A | C |

# Fig. 19: A-18

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1242 | C | PRO | 310 | 138.569 | 32.751 | -3.178 | 1.00 | 20.19 | A | C |
| ATOM | 1243 | O | PRO | 310 | 138.229 | 33.654 | -2.394 | 1.00 | 16.98 | A | O |
| ATOM | 1244 | N | THR | 311 | 138.197 | 31.483 | -3.043 | 1.00 | 25.93 | A | N |
| ATOM | 1245 | CA | THR | 311 | 137.352 | 31.013 | -1.957 | 1.00 | 26.80 | A | C |
| ATOM | 1246 | CB | THR | 311 | 137.618 | 29.521 | -1.695 | 1.00 | 73.61 | A | C |
| ATOM | 1247 | OG1 | THR | 311 | 137.053 | 29.145 | -0.434 | 1.00 | 77.77 | A | O |
| ATOM | 1248 | CG2 | THR | 311 | 139.118 | 29.244 | -1.696 | 1.00 | 76.69 | A | C |
| ATOM | 1249 | C | THR | 311 | 137.521 | 31.781 | -0.643 | 1.00 | 28.67 | A | C |
| ATOM | 1250 | O | THR | 311 | 136.535 | 32.173 | -0.025 | 1.00 | 29.84 | A | O |
| ATOM | 1251 | N | GLU | 312 | 138.759 | 32.009 | -0.223 | 1.00 | 47.89 | A | N |
| ATOM | 1252 | CA | GLU | 312 | 139.007 | 32.713 | 1.029 | 1.00 | 46.51 | A | C |
| ATOM | 1253 | CB | GLU | 312 | 140.506 | 32.751 | 1.340 | 1.00 | 98.24 | A | C |
| ATOM | 1254 | CG | GLU | 312 | 141.354 | 33.411 | 0.268 | 1.00 | 100.00 | A | C |
| ATOM | 1255 | CD | GLU | 312 | 142.621 | 34.031 | 0.825 | 1.00 | 99.11 | A | C |
| ATOM | 1256 | OE1 | GLU | 312 | 143.491 | 34.431 | 0.024 | 1.00 | 102.46 | A | O |
| ATOM | 1257 | OE2 | GLU | 312 | 142.742 | 34.130 | 2.065 | 1.00 | 99.98 | A | O |
| ATOM | 1258 | C | GLU | 312 | 138.453 | 34.134 | 1.092 | 1.00 | 45.13 | A | C |
| ATOM | 1259 | O | GLU | 312 | 137.997 | 34.576 | 2.147 | 1.00 | 45.09 | A | O |
| ATOM | 1260 | N | LYS | 313 | 138.490 | 34.856 | -0.021 | 1.00 | 49.11 | A | N |
| ATOM | 1261 | CA | LYS | 313 | 137.990 | 36.226 | -0.024 | 1.00 | 48.31 | A | C |
| ATOM | 1262 | CB | LYS | 313 | 138.797 | 37.091 | -1.000 | 1.00 | 91.02 | A | C |
| ATOM | 1263 | CG | LYS | 313 | 140.171 | 37.508 | -0.486 | 1.00 | 90.90 | A | C |
| ATOM | 1264 | CD | LYS | 313 | 140.081 | 38.565 | 0.620 | 1.00 | 87.20 | A | C |
| ATOM | 1265 | CE | LYS | 313 | 139.966 | 39.982 | 0.066 | 1.00 | 89.24 | A | C |
| ATOM | 1266 | NZ | LYS | 313 | 138.804 | 40.159 | -0.842 | 1.00 | 93.72 | A | N |
| ATOM | 1267 | C | LYS | 313 | 136.511 | 36.307 | -0.374 | 1.00 | 49.46 | A | C |
| ATOM | 1268 | O | LYS | 313 | 135.973 | 37.397 | -0.580 | 1.00 | 51.78 | A | O |
| ATOM | 1269 | N | HIS | 314 | 135.849 | 35.159 | -0.427 | 1.00 | 27.67 | A | N |
| ATOM | 1270 | CA | HIS | 314 | 134.437 | 35.137 | -0.775 | 1.00 | 28.52 | A | C |
| ATOM | 1271 | CB | HIS | 314 | 134.274 | 34.652 | -2.212 | 1.00 | 32.51 | A | C |
| ATOM | 1272 | CG | HIS | 314 | 134.872 | 35.574 | -3.224 | 1.00 | 29.37 | A | C |
| ATOM | 1273 | CD2 | HIS | 314 | 136.073 | 35.552 | -3.849 | 1.00 | 28.84 | A | C |
| ATOM | 1274 | ND1 | HIS | 314 | 134.220 | 36.697 | -3.683 | 1.00 | 28.95 | A | N |
| ATOM | 1275 | CE1 | HIS | 314 | 134.992 | 37.326 | -4.551 | 1.00 | 28.24 | A | C |
| ATOM | 1276 | NE2 | HIS | 314 | 136.122 | 36.652 | -4.669 | 1.00 | 28.63 | A | N |
| ATOM | 1277 | C | HIS | 314 | 133.587 | 34.277 | 0.141 | 1.00 | 28.65 | A | C |
| ATOM | 1278 | O | HIS | 314 | 132.366 | 34.238 | -0.008 | 1.00 | 32.05 | A | O |
| ATOM | 1279 | N | PHE | 315 | 134.230 | 33.591 | 1.081 | 1.00 | 32.99 | A | N |
| ATOM | 1280 | CA | PHE | 315 | 133.519 | 32.723 | 2.013 | 1.00 | 32.79 | A | C |
| ATOM | 1281 | CB | PHE | 315 | 134.045 | 31.294 | 1.878 | 1.00 | 35.38 | A | C |
| ATOM | 1282 | CG | PHE | 315 | 133.476 | 30.339 | 2.884 | 1.00 | 30.36 | A | C |
| ATOM | 1283 | CD1 | PHE | 315 | 132.123 | 30.026 | 2.877 | 1.00 | 32.20 | A | C |
| ATOM | 1284 | CD2 | PHE | 315 | 134.298 | 29.749 | 3.839 | 1.00 | 28.44 | A | C |
| ATOM | 1285 | CE1 | PHE | 315 | 131.592 | 29.144 | 3.800 | 1.00 | 27.15 | A | C |
| ATOM | 1286 | CE2 | PHE | 315 | 133.783 | 28.866 | 4.769 | 1.00 | 29.14 | A | C |
| ATOM | 1287 | CZ | PHE | 315 | 132.421 | 28.560 | 4.749 | 1.00 | 30.81 | A | C |
| ATOM | 1288 | C | PHE | 315 | 133.640 | 33.198 | 3.466 | 1.00 | 33.51 | A | C |
| ATOM | 1289 | O | PHE | 315 | 134.706 | 33.643 | 3.896 | 1.00 | 34.91 | A | O |
| ATOM | 1290 | N | PHE | 316 | 132.539 | 33.104 | 4.210 | 1.00 | 26.09 | A | N |
| ATOM | 1291 | CA | PHE | 316 | 132.513 | 33.516 | 5.610 | 1.00 | 23.14 | A | C |
| ATOM | 1292 | CB | PHE | 316 | 131.707 | 34.803 | 5.780 | 1.00 | 27.51 | A | C |
| ATOM | 1293 | CG | PHE | 316 | 132.343 | 36.008 | 5.155 | 1.00 | 31.13 | A | C |
| ATOM | 1294 | CD1 | PHE | 316 | 132.125 | 36.312 | 3.822 | 1.00 | 26.72 | A | C |
| ATOM | 1295 | CD2 | PHE | 316 | 133.182 | 36.827 | 5.903 | 1.00 | 27.98 | A | C |
| ATOM | 1296 | CE1 | PHE | 316 | 132.737 | 37.420 | 3.237 | 1.00 | 29.29 | A | C |
| ATOM | 1297 | CE2 | PHE | 316 | 133.799 | 37.931 | 5.334 | 1.00 | 31.09 | A | C |
| ATOM | 1298 | CZ | PHE | 316 | 133.577 | 38.230 | 3.998 | 1.00 | 31.32 | A | C |
| ATOM | 1299 | C | PHE | 316 | 131.909 | 32.438 | 6.497 | 1.00 | 21.07 | A | C |
| ATOM | 1300 | O | PHE | 316 | 130.901 | 31.831 | 6.153 | 1.00 | 20.31 | A | O |
| ATOM | 1301 | N | ASN | 317 | 132.533 | 32.220 | 7.647 | 1.00 | 37.16 | A | N |
| ATOM | 1302 | CA | ASN | 317 | 132.093 | 31.214 | 8.599 | 1.00 | 38.38 | A | C |
| ATOM | 1303 | CB | ASN | 317 | 133.288 | 30.385 | 9.047 | 1.00 | 74.28 | A | C |
| ATOM | 1304 | CG | ASN | 317 | 133.055 | 28.919 | 8.888 | 1.00 | 77.27 | A | C |
| ATOM | 1305 | OD1 | ASN | 317 | 131.954 | 28.433 | 9.138 | 1.00 | 79.20 | A | O |
| ATOM | 1306 | ND2 | ASN | 317 | 134.088 | 28.190 | 8.478 | 1.00 | 75.53 | A | N |
| ATOM | 1307 | C | ASN | 317 | 131.487 | 31.893 | 9.817 | 1.00 | 39.34 | A | C |
| ATOM | 1308 | O | ASN | 317 | 132.001 | 32.902 | 10.285 | 1.00 | 40.20 | A | O |
| ATOM | 1309 | N | VAL | 318 | 130.398 | 31.348 | 10.336 | 1.00 | 30.64 | A | N |
| ATOM | 1310 | CA | VAL | 318 | 129.763 | 31.924 | 11.521 | 1.00 | 29.27 | A | C |
| ATOM | 1311 | CB | VAL | 318 | 128.531 | 32.778 | 11.144 | 1.00 | 70.89 | A | C |
| ATOM | 1312 | CG1 | VAL | 318 | 127.896 | 33.349 | 12.386 | 1.00 | 71.02 | A | C |
| ATOM | 1313 | CG2 | VAL | 318 | 128.942 | 33.899 | 10.223 | 1.00 | 70.87 | A | C |
| ATOM | 1314 | C | VAL | 318 | 129.331 | 30.808 | 12.482 | 1.00 | 24.42 | A | C |

# Fig. 19: A-19

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1315 | O | VAL | 318 | 128.872 | 29.744 | 12.053 | 1.00 | 25.09 | A | O |
| ATOM | 1316 | N | SER | 319 | 129.482 | 31.045 | 13.779 | 1.00 | 32.47 | A | N |
| ATOM | 1317 | CA | SER | 319 | 129.108 | 30.035 | 14.752 | 1.00 | 31.73 | A | C |
| ATOM | 1318 | CB | SER | 319 | 129.669 | 30.384 | 16.134 | 1.00 | 29.19 | A | C |
| ATOM | 1319 | OG | SER | 319 | 129.289 | 31.687 | 16.538 | 1.00 | 41.14 | A | O |
| ATOM | 1320 | C | SER | 319 | 127.600 | 29.840 | 14.831 | 1.00 | 30.33 | A | C |
| ATOM | 1321 | O | SER | 319 | 127.132 | 28.716 | 14.963 | 1.00 | 28.40 | A | O |
| ATOM | 1322 | N | ASP | 320 | 126.839 | 30.926 | 14.741 | 1.00 | 32.33 | A | N |
| ATOM | 1323 | CA | ASP | 320 | 125.382 | 30.846 | 14.816 | 1.00 | 32.31 | A | C |
| ATOM | 1324 | CB | ASP | 320 | 124.934 | 30.632 | 16.275 | 1.00 | 63.91 | A | C |
| ATOM | 1325 | CG | ASP | 320 | 125.369 | 31.760 | 17.209 | 1.00 | 62.36 | A | C |
| ATOM | 1326 | OD1 | ASP | 320 | 126.586 | 31.992 | 17.364 | 1.00 | 61.04 | A | O |
| ATOM | 1327 | OD2 | ASP | 320 | 124.486 | 32.412 | 17.801 | 1.00 | 62.91 | A | O |
| ATOM | 1328 | C | ASP | 320 | 124.698 | 32.088 | 14.237 | 1.00 | 30.68 | A | C |
| ATOM | 1329 | O | ASP | 320 | 125.367 | 33.072 | 13.905 | 1.00 | 30.46 | A | O |
| ATOM | 1330 | N | GLU | 321 | 123.371 | 32.042 | 14.110 | 1.00 | 35.58 | A | N |
| ATOM | 1331 | CA | GLU | 321 | 122.614 | 33.173 | 13.569 | 1.00 | 36.56 | A | C |
| ATOM | 1332 | CB | GLU | 321 | 121.126 | 33.029 | 13.889 | 1.00 | 84.00 | A | C |
| ATOM | 1333 | CG | GLU | 321 | 120.285 | 32.398 | 12.796 | 1.00 | 77.84 | A | C |
| ATOM | 1334 | CD | GLU | 321 | 120.602 | 30.938 | 12.569 | 1.00 | 77.59 | A | C |
| ATOM | 1335 | OE1 | GLU | 321 | 120.595 | 30.164 | 13.549 | 1.00 | 79.02 | A | O |
| ATOM | 1336 | OE2 | GLU | 321 | 120.849 | 30.565 | 11.404 | 1.00 | 81.63 | A | O |
| ATOM | 1337 | C | GLU | 321 | 123.101 | 34.500 | 14.134 | 1.00 | 40.55 | A | C |
| ATOM | 1338 | O | GLU | 321 | 123.278 | 35.475 | 13.397 | 1.00 | 37.31 | A | O |
| ATOM | 1339 | N | LEU | 322 | 123.323 | 34.519 | 15.447 | 1.00 | 25.97 | A | N |
| ATOM | 1340 | CA | LEU | 322 | 123.769 | 35.717 | 16.155 | 1.00 | 28.66 | A | C |
| ATOM | 1341 | CB | LEU | 322 | 123.925 | 35.407 | 17.648 | 1.00 | 49.06 | A | C |
| ATOM | 1342 | CG | LEU | 322 | 122.646 | 35.281 | 18.477 | 1.00 | 47.69 | A | C |
| ATOM | 1343 | CD1 | LEU | 322 | 121.935 | 36.625 | 18.486 | 1.00 | 49.43 | A | C |
| ATOM | 1344 | CD2 | LEU | 322 | 121.745 | 34.194 | 17.917 | 1.00 | 52.74 | A | C |
| ATOM | 1345 | C | LEU | 322 | 125.052 | 36.368 | 15.644 | 1.00 | 30.25 | A | C |
| ATOM | 1346 | O | LEU | 322 | 125.106 | 37.580 | 15.459 | 1.00 | 33.60 | A | O |
| ATOM | 1347 | N | ALA | 323 | 126.080 | 35.558 | 15.424 | 1.00 | 27.12 | A | N |
| ATOM | 1348 | CA | ALA | 323 | 127.358 | 36.071 | 14.965 | 1.00 | 27.55 | A | C |
| ATOM | 1349 | CB | ALA | 323 | 128.420 | 34.994 | 15.112 | 1.00 | 20.92 | A | C |
| ATOM | 1350 | C | ALA | 323 | 127.368 | 36.631 | 13.539 | 1.00 | 27.96 | A | C |
| ATOM | 1351 | O | ALA | 323 | 128.363 | 37.227 | 13.120 | 1.00 | 27.98 | A | O |
| ATOM | 1352 | N | LEU | 324 | 126.280 | 36.451 | 12.794 | 1.00 | 44.60 | A | N |
| ATOM | 1353 | CA | LEU | 324 | 126.231 | 36.961 | 11.427 | 1.00 | 43.08 | A | C |
| ATOM | 1354 | CB | LEU | 324 | 124.807 | 36.875 | 10.867 | 1.00 | 12.96 | A | C |
| ATOM | 1355 | CG | LEU | 324 | 124.398 | 35.546 | 10.215 | 1.00 | 11.69 | A | C |
| ATOM | 1356 | CD1 | LEU | 324 | 122.900 | 35.547 | 9.935 | 1.00 | 10.83 | A | C |
| ATOM | 1357 | CD2 | LEU | 324 | 125.197 | 35.331 | 8.938 | 1.00 | 9.62 | A | C |
| ATOM | 1358 | C | LEU | 324 | 126.734 | 38.400 | 11.346 | 1.00 | 46.61 | A | C |
| ATOM | 1359 | O | LEU | 324 | 127.545 | 38.735 | 10.484 | 1.00 | 43.15 | A | O |
| ATOM | 1360 | N | VAL | 325 | 126.257 | 39.244 | 12.252 | 1.00 | 37.14 | A | N |
| ATOM | 1361 | CA | VAL | 325 | 126.657 | 40.645 | 12.297 | 1.00 | 40.67 | A | C |
| ATOM | 1362 | CB | VAL | 325 | 126.111 | 41.328 | 13.549 | 1.00 | 15.02 | A | C |
| ATOM | 1363 | CG1 | VAL | 325 | 124.613 | 41.517 | 13.425 | 1.00 | 15.13 | A | C |
| ATOM | 1364 | CG2 | VAL | 325 | 126.453 | 40.503 | 14.773 | 1.00 | 18.41 | A | C |
| ATOM | 1365 | C | VAL | 325 | 128.168 | 40.840 | 12.304 | 1.00 | 43.49 | A | C |
| ATOM | 1366 | O | VAL | 325 | 128.706 | 41.663 | 11.560 | 1.00 | 45.55 | A | O |
| ATOM | 1367 | N | THR | 326 | 128.844 | 40.088 | 13.161 | 1.00 | 37.74 | A | N |
| ATOM | 1368 | CA | THR | 326 | 130.289 | 40.164 | 13.286 | 1.00 | 39.15 | A | C |
| ATOM | 1369 | CB | THR | 326 | 130.768 | 39.218 | 14.391 | 1.00 | 28.63 | A | C |
| ATOM | 1370 | OG1 | THR | 326 | 130.648 | 37.863 | 13.944 | 1.00 | 30.54 | A | O |
| ATOM | 1371 | CG2 | THR | 326 | 129.911 | 39.398 | 15.643 | 1.00 | 31.00 | A | C |
| ATOM | 1372 | C | THR | 326 | 130.996 | 39.790 | 11.985 | 1.00 | 39.16 | A | C |
| ATOM | 1373 | O | THR | 326 | 132.105 | 39.268 | 12.005 | 1.00 | 37.98 | A | O |
| ATOM | 1374 | N | ILE | 327 | 130.358 | 40.065 | 10.854 | 1.00 | 29.50 | A | N |
| ATOM | 1375 | CA | ILE | 327 | 130.922 | 39.739 | 9.552 | 1.00 | 29.69 | A | C |
| ATOM | 1376 | CB | ILE | 327 | 130.407 | 38.343 | 9.098 | 1.00 | 36.77 | A | C |
| ATOM | 1377 | CG2 | ILE | 327 | 129.867 | 38.372 | 7.679 | 1.00 | 37.54 | A | C |
| ATOM | 1378 | CG1 | ILE | 327 | 131.539 | 37.335 | 9.199 | 1.00 | 37.13 | A | C |
| ATOM | 1379 | CD1 | ILE | 327 | 131.100 | 35.928 | 8.903 | 1.00 | 36.80 | A | C |
| ATOM | 1380 | C | ILE | 327 | 130.572 | 40.816 | 8.520 | 1.00 | 30.20 | A | C |
| ATOM | 1381 | O | ILE | 327 | 131.284 | 41.008 | 7.530 | 1.00 | 30.45 | A | O |
| ATOM | 1382 | N | VAL | 328 | 129.478 | 41.527 | 8.766 | 1.00 | 25.26 | A | N |
| ATOM | 1383 | CA | VAL | 328 | 129.040 | 42.565 | 7.851 | 1.00 | 27.40 | A | C |
| ATOM | 1384 | CB | VAL | 328 | 127.851 | 43.363 | 8.436 | 1.00 | 56.37 | A | C |
| ATOM | 1385 | CG1 | VAL | 328 | 126.752 | 42.408 | 8.838 | 1.00 | 58.32 | A | C |
| ATOM | 1386 | CG2 | VAL | 328 | 128.301 | 44.197 | 9.626 | 1.00 | 57.64 | A | C |
| ATOM | 1387 | C | VAL | 328 | 130.159 | 43.539 | 7.485 | 1.00 | 27.32 | A | C |

# Fig. 19: A-20

| | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1388 | O | VAL | 328 | 130.220 | 44.017 | 6.355 | 1.00 | 26.60 | A | O |
| ATOM | 1389 | N | LYS | 329 | 131.047 | 43.837 | 8.426 | 1.00 | 32.39 | A | N |
| ATOM | 1390 | CA | LYS | 329 | 132.121 | 44.773 | 8.124 | 1.00 | 31.60 | A | C |
| ATOM | 1391 | CB | LYS | 329 | 132.949 | 45.076 | 9.378 | 1.00 | 67.11 | A | C |
| ATOM | 1392 | CG | LYS | 329 | 133.861 | 46.291 | 9.242 | 1.00 | 68.66 | A | C |
| ATOM | 1393 | CD | LYS | 329 | 134.737 | 46.454 | 10.474 | 1.00 | 70.98 | A | C |
| ATOM | 1394 | CE | LYS | 329 | 135.540 | 47.746 | 10.437 | 1.00 | 74.02 | A | C |
| ATOM | 1395 | NZ | LYS | 329 | 134.660 | 48.952 | 10.496 | 1.00 | 77.70 | A | N |
| ATOM | 1396 | C | LYS | 329 | 133.014 | 44.194 | 7.036 | 1.00 | 29.77 | A | C |
| ATOM | 1397 | O | LYS | 329 | 133.205 | 44.802 | 5.978 | 1.00 | 30.98 | A | O |
| ATOM | 1398 | N | ALA | 330 | 133.551 | 43.008 | 7.293 | 1.00 | 29.12 | A | N |
| ATOM | 1399 | CA | ALA | 330 | 134.425 | 42.365 | 6.331 | 1.00 | 29.15 | A | C |
| ATOM | 1400 | CB | ALA | 330 | 134.997 | 41.091 | 6.922 | 1.00 | 30.19 | A | C |
| ATOM | 1401 | C | ALA | 330 | 133.681 | 42.056 | 5.043 | 1.00 | 30.30 | A | C |
| ATOM | 1402 | O | ALA | 330 | 134.207 | 42.269 | 3.955 | 1.00 | 30.20 | A | O |
| ATOM | 1403 | N | LEU | 331 | 132.457 | 41.551 | 5.168 | 1.00 | 22.22 | A | N |
| ATOM | 1404 | CA | LEU | 331 | 131.661 | 41.206 | 3.994 | 1.00 | 19.86 | A | C |
| ATOM | 1405 | CB | LEU | 331 | 130.284 | 40.667 | 4.403 | 1.00 | 36.97 | A | C |
| ATOM | 1406 | CG | LEU | 331 | 129.567 | 39.761 | 3.389 | 1.00 | 33.39 | A | C |
| ATOM | 1407 | CD1 | LEU | 331 | 128.110 | 39.600 | 3.787 | 1.00 | 35.02 | A | C |
| ATOM | 1408 | CD2 | LEU | 331 | 129.658 | 40.343 | 1.996 | 1.00 | 29.08 | A | C |
| ATOM | 1409 | C | LEU | 331 | 131.483 | 42.467 | 3.162 | 1.00 | 19.89 | A | C |
| ATOM | 1410 | O | LEU | 331 | 131.741 | 42.468 | 1.961 | 1.00 | 19.24 | A | O |
| ATOM | 1411 | N | GLY | 332 | 131.045 | 43.535 | 3.830 | 1.00 | 15.82 | A | N |
| ATOM | 1412 | CA | GLY | 332 | 130.824 | 44.811 | 3.179 | 1.00 | 16.92 | A | C |
| ATOM | 1413 | C | GLY | 332 | 132.024 | 45.309 | 2.402 | 1.00 | 17.18 | A | C |
| ATOM | 1414 | O | GLY | 332 | 131.911 | 45.651 | 1.224 | 1.00 | 21.05 | A | O |
| ATOM | 1415 | N | GLU | 333 | 133.185 | 45.347 | 3.045 | 1.00 | 34.74 | A | N |
| ATOM | 1416 | CA | GLU | 333 | 134.369 | 45.831 | 2.362 | 1.00 | 32.80 | A | C |
| ATOM | 1417 | CB | GLU | 333 | 135.472 | 46.165 | 3.371 | 1.00 | 75.29 | A | C |
| ATOM | 1418 | CG | GLU | 333 | 136.139 | 44.968 | 4.005 | 1.00 | 73.66 | A | C |
| ATOM | 1419 | CD | GLU | 333 | 137.251 | 45.363 | 4.959 | 1.00 | 73.68 | A | C |
| ATOM | 1420 | OE1 | GLU | 333 | 137.953 | 44.459 | 5.456 | 1.00 | 75.73 | A | O |
| ATOM | 1421 | OE2 | GLU | 333 | 137.421 | 46.575 | 5.215 | 1.00 | 67.80 | A | O |
| ATOM | 1422 | C | GLU | 333 | 134.888 | 44.841 | 1.322 | 1.00 | 31.78 | A | C |
| ATOM | 1423 | O | GLU | 333 | 135.370 | 45.236 | 0.261 | 1.00 | 31.40 | A | O |
| ATOM | 1424 | N | ARG | 334 | 134.781 | 43.552 | 1.610 | 1.00 | 50.02 | A | N |
| ATOM | 1425 | CA | ARG | 334 | 135.275 | 42.563 | 0.669 | 1.00 | 53.40 | A | C |
| ATOM | 1426 | CB | ARG | 334 | 135.064 | 41.152 | 1.215 | 1.00 | 83.27 | A | C |
| ATOM | 1427 | CG | ARG | 334 | 136.000 | 40.123 | 0.607 | 1.00 | 82.56 | A | C |
| ATOM | 1428 | CD | ARG | 334 | 136.564 | 39.198 | 1.677 | 1.00 | 81.32 | A | C |
| ATOM | 1429 | NE | ARG | 334 | 137.441 | 39.901 | 2.612 | 1.00 | 76.87 | A | N |
| ATOM | 1430 | CZ | ARG | 334 | 137.888 | 39.383 | 3.753 | 1.00 | 80.96 | A | C |
| ATOM | 1431 | NH1 | ARG | 334 | 137.537 | 38.148 | 4.108 | 1.00 | 77.70 | A | N |
| ATOM | 1432 | NH2 | ARG | 334 | 138.686 | 40.097 | 4.539 | 1.00 | 87.10 | A | N |
| ATOM | 1433 | C | ARG | 334 | 134.556 | 42.757 | -0.654 | 1.00 | 54.70 | A | C |
| ATOM | 1434 | O | ARG | 334 | 135.170 | 42.716 | -1.716 | 1.00 | 51.62 | A | O |
| ATOM | 1435 | N | ILE | 335 | 133.253 | 42.988 | -0.591 | 1.00 | 36.48 | A | N |
| ATOM | 1436 | CA | ILE | 335 | 132.473 | 43.214 | -1.803 | 1.00 | 36.41 | A | C |
| ATOM | 1437 | CB | ILE | 335 | 130.940 | 42.967 | -1.539 | 1.00 | 33.09 | A | C |
| ATOM | 1438 | CG2 | ILE | 335 | 130.524 | 43.522 | -0.203 | 1.00 | 35.87 | A | C |
| ATOM | 1439 | CG1 | ILE | 335 | 130.094 | 43.611 | -2.630 | 1.00 | 34.31 | A | C |
| ATOM | 1440 | CD1 | ILE | 335 | 128.612 | 43.520 | -2.368 | 1.00 | 37.10 | A | C |
| ATOM | 1441 | C | ILE | 335 | 132.742 | 44.663 | -2.215 | 1.00 | 34.70 | A | C |
| ATOM | 1442 | O | ILE | 335 | 132.421 | 45.092 | -3.326 | 1.00 | 37.30 | A | O |
| ATOM | 1443 | N | PHE | 336 | 133.392 | 45.377 | -1.299 | 1.00 | 108.43 | A | N |
| ATOM | 1444 | CA | PHE | 336 | 133.744 | 46.789 | -1.419 | 1.00 | 108.06 | A | C |
| ATOM | 1445 | CB | PHE | 336 | 135.092 | 46.989 | -2.157 | 1.00 | 57.00 | A | C |
| ATOM | 1446 | CG | PHE | 336 | 135.114 | 46.540 | -3.601 | 1.00 | 53.32 | A | C |
| ATOM | 1447 | CD1 | PHE | 336 | 134.135 | 46.941 | -4.508 | 1.00 | 52.74 | A | C |
| ATOM | 1448 | CD2 | PHE | 336 | 136.178 | 45.779 | -4.073 | 1.00 | 51.27 | A | C |
| ATOM | 1449 | CE1 | PHE | 336 | 134.219 | 46.589 | -5.868 | 1.00 | 43.07 | A | C |
| ATOM | 1450 | CE2 | PHE | 336 | 136.271 | 45.426 | -5.422 | 1.00 | 45.63 | A | C |
| ATOM | 1451 | CZ | PHE | 336 | 135.292 | 45.832 | -6.319 | 1.00 | 46.09 | A | C |
| ATOM | 1452 | C | PHE | 336 | 132.662 | 47.670 | -2.020 | 1.00 | 108.09 | A | C |
| ATOM | 1453 | O | PHE | 336 | 131.623 | 47.131 | -2.453 | 1.00 | 87.71 | A | O |
| ATOM | 1454 | OXT | PHE | 336 | 132.864 | 48.902 | -2.024 | 1.00 | 40.49 | A | O |
| ATOM | 1455 | CB | GLU | 1 | 119.537 | 12.185 | 27.786 | 1.00 | 88.08 | H | C |
| ATOM | 1456 | CG | GLU | 1 | 118.650 | 11.120 | 28.419 | 1.00 | 88.08 | H | C |
| ATOM | 1457 | CD | GLU | 1 | 119.399 | 10.237 | 29.409 | 1.00 | 88.08 | H | C |
| ATOM | 1458 | OE1 | GLU | 1 | 120.127 | 10.777 | 30.271 | 1.00 | 88.08 | H | O |
| ATOM | 1459 | OE2 | GLU | 1 | 119.251 | 8.998 | 29.324 | 1.00 | 88.08 | H | O |
| ATOM | 1460 | C | GLU | 1 | 118.366 | 14.360 | 28.176 | 1.00 | 62.78 | H | C |

Fig. 19: A-21

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1461 | O | GLU | 1 | 117.763 | 15.033 | 29.012 | 1.00 | 62.78 | H | O |
| ATOM | 1462 | N | GLU | 1 | 119.687 | 13.262 | 30.016 | 1.00 | 62.78 | H | N |
| ATOM | 1463 | CA | GLU | 1 | 119.580 | 13.515 | 28.553 | 1.00 | 62.78 | H | C |
| ATOM | 1464 | N | VAL | 2 | 118.019 | 14.312 | 26.896 | 1.00 | 44.26 | H | N |
| ATOM | 1465 | CA | VAL | 2 | 116.896 | 15.064 | 26.359 | 1.00 | 44.26 | H | C |
| ATOM | 1466 | CB | VAL | 2 | 117.154 | 15.460 | 24.909 | 1.00 | 15.14 | H | C |
| ATOM | 1467 | CG1 | VAL | 2 | 118.610 | 15.840 | 24.732 | 1.00 | 15.14 | H | C |
| ATOM | 1468 | CG2 | VAL | 2 | 116.807 | 14.309 | 23.997 | 1.00 | 15.14 | H | C |
| ATOM | 1469 | C | VAL | 2 | 115.677 | 14.174 | 26.353 | 1.00 | 44.26 | H | C |
| ATOM | 1470 | O | VAL | 2 | 115.803 | 12.951 | 26.347 | 1.00 | 44.26 | H | O |
| ATOM | 1471 | N | GLN | 3 | 114.497 | 14.780 | 26.340 | 1.00 | 25.45 | H | N |
| ATOM | 1472 | CA | GLN | 3 | 113.280 | 13.984 | 26.288 | 1.00 | 25.45 | H | C |
| ATOM | 1473 | CB | GLN | 3 | 113.191 | 13.046 | 27.494 | 1.00 | 105.15 | H | C |
| ATOM | 1474 | CG | GLN | 3 | 113.307 | 13.707 | 28.841 | 1.00 | 105.15 | H | C |
| ATOM | 1475 | CD | GLN | 3 | 113.015 | 12.733 | 29.961 | 1.00 | 105.15 | H | C |
| ATOM | 1476 | OE1 | GLN | 3 | 113.554 | 11.623 | 29.990 | 1.00 | 105.15 | H | O |
| ATOM | 1477 | NE2 | GLN | 3 | 112.157 | 13.139 | 30.892 | 1.00 | 105.15 | H | N |
| ATOM | 1478 | C | GLN | 3 | 111.961 | 14.708 | 26.119 | 1.00 | 25.45 | H | C |
| ATOM | 1479 | O | GLN | 3 | 111.809 | 15.887 | 26.438 | 1.00 | 25.45 | H | O |
| ATOM | 1480 | N | LEU | 4 | 111.009 | 13.959 | 25.588 | 1.00 | 27.88 | H | N |
| ATOM | 1481 | CA | LEU | 4 | 109.668 | 14.446 | 25.339 | 1.00 | 27.88 | H | C |
| ATOM | 1482 | CB | LEU | 4 | 109.347 | 14.369 | 23.842 | 1.00 | 33.14 | H | C |
| ATOM | 1483 | CG | LEU | 4 | 110.367 | 14.924 | 22.847 | 1.00 | 33.14 | H | C |
| ATOM | 1484 | CD1 | LEU | 4 | 109.821 | 14.772 | 21.438 | 1.00 | 33.14 | H | C |
| ATOM | 1485 | CD2 | LEU | 4 | 110.646 | 16.385 | 23.155 | 1.00 | 33.14 | H | C |
| ATOM | 1486 | C | LEU | 4 | 108.755 | 13.507 | 26.095 | 1.00 | 27.88 | H | C |
| ATOM | 1487 | O | LEU | 4 | 108.871 | 12.282 | 25.960 | 1.00 | 27.88 | H | O |
| ATOM | 1488 | N | VAL | 5 | 107.858 | 14.061 | 26.901 | 1.00 | 26.47 | H | N |
| ATOM | 1489 | CA | VAL | 5 | 106.942 | 13.215 | 27.656 | 1.00 | 26.47 | H | C |
| ATOM | 1490 | CB | VAL | 5 | 107.176 | 13.329 | 29.197 | 1.00 | 25.39 | H | C |
| ATOM | 1491 | CG1 | VAL | 5 | 107.281 | 14.772 | 29.606 | 1.00 | 25.39 | H | C |
| ATOM | 1492 | CG2 | VAL | 5 | 106.046 | 12.654 | 29.947 | 1.00 | 25.39 | H | C |
| ATOM | 1493 | C | VAL | 5 | 105.520 | 13.578 | 27.297 | 1.00 | 26.47 | H | C |
| ATOM | 1494 | O | VAL | 5 | 105.031 | 14.664 | 27.635 | 1.00 | 26.47 | H | O |
| ATOM | 1495 | N | GLU | 6 | 104.868 | 12.650 | 26.601 | 1.00 | 23.78 | H | N |
| ATOM | 1496 | CA | GLU | 6 | 103.495 | 12.835 | 26.133 | 1.00 | 23.78 | H | C |
| ATOM | 1497 | CB | GLU | 6 | 103.258 | 11.995 | 24.885 | 1.00 | 29.58 | H | C |
| ATOM | 1498 | CG | GLU | 6 | 104.409 | 12.017 | 23.933 | 1.00 | 29.58 | H | C |
| ATOM | 1499 | CD | GLU | 6 | 104.188 | 11.109 | 22.756 | 1.00 | 29.58 | H | C |
| ATOM | 1500 | OE1 | GLU | 6 | 105.194 | 10.664 | 22.168 | 1.00 | 29.58 | H | O |
| ATOM | 1501 | OE2 | GLU | 6 | 103.013 | 10.846 | 22.413 | 1.00 | 29.58 | H | O |
| ATOM | 1502 | C | GLU | 6 | 102.429 | 12.485 | 27.155 | 1.00 | 23.78 | H | C |
| ATOM | 1503 | O | GLU | 6 | 102.680 | 11.740 | 28.101 | 1.00 | 23.78 | H | O |
| ATOM | 1504 | N | SER | 7 | 101.242 | 13.047 | 26.937 | 1.00 | 26.30 | H | N |
| ATOM | 1505 | CA | SER | 7 | 100.061 | 12.823 | 27.766 | 1.00 | 26.30 | H | C |
| ATOM | 1506 | CB | SER | 7 | 100.177 | 13.535 | 29.102 | 1.00 | 32.56 | H | C |
| ATOM | 1507 | OG | SER | 7 | 100.574 | 14.871 | 28.906 | 1.00 | 32.56 | H | O |
| ATOM | 1508 | C | SER | 7 | 98.886 | 13.381 | 26.998 | 1.00 | 26.30 | H | C |
| ATOM | 1509 | O | SER | 7 | 99.060 | 14.248 | 26.136 | 1.00 | 26.30 | H | O |
| ATOM | 1510 | N | GLY | 8 | 97.693 | 12.872 | 27.287 | 1.00 | 41.74 | H | N |
| ATOM | 1511 | CA | GLY | 8 | 96.514 | 13.360 | 26.598 | 1.00 | 41.74 | H | C |
| ATOM | 1512 | C | GLY | 8 | 95.807 | 12.321 | 25.752 | 1.00 | 41.74 | H | C |
| ATOM | 1513 | O | GLY | 8 | 94.745 | 12.603 | 25.201 | 1.00 | 41.74 | H | O |
| ATOM | 1514 | N | GLY | 9 | 96.383 | 11.127 | 25.637 | 1.00 | 47.50 | H | N |
| ATOM | 1515 | CA | GLY | 9 | 95.751 | 10.079 | 24.851 | 1.00 | 47.50 | H | C |
| ATOM | 1516 | C | GLY | 9 | 94.431 | 9.601 | 25.446 | 1.00 | 47.50 | H | C |
| ATOM | 1517 | O | GLY | 9 | 94.038 | 10.020 | 26.536 | 1.00 | 47.50 | H | O |
| ATOM | 1518 | N | GLY | 10 | 93.732 | 8.723 | 24.735 | 1.00 | 16.50 | H | N |
| ATOM | 1519 | CA | GLY | 10 | 92.469 | 8.225 | 25.244 | 1.00 | 16.50 | H | C |
| ATOM | 1520 | C | GLY | 10 | 91.485 | 7.806 | 24.169 | 1.00 | 16.50 | H | C |
| ATOM | 1521 | O | GLY | 10 | 91.830 | 7.701 | 22.990 | 1.00 | 16.50 | H | O |
| ATOM | 1522 | N | LEU | 11 | 90.251 | 7.559 | 24.595 | 1.00 | 37.61 | H | N |
| ATOM | 1523 | CA | LEU | 11 | 89.175 | 7.137 | 23.710 | 1.00 | 37.61 | H | C |
| ATOM | 1524 | CB | LEU | 11 | 88.388 | 6.003 | 24.365 | 1.00 | 18.32 | H | C |
| ATOM | 1525 | CG | LEU | 11 | 86.959 | 5.715 | 23.885 | 1.00 | 18.32 | H | C |
| ATOM | 1526 | CD1 | LEU | 11 | 86.962 | 5.148 | 22.463 | 1.00 | 18.32 | H | C |
| ATOM | 1527 | CD2 | LEU | 11 | 86.313 | 4.729 | 24.856 | 1.00 | 18.32 | H | C |
| ATOM | 1528 | C | LEU | 11 | 88.235 | 8.292 | 23.436 | 1.00 | 37.61 | H | C |
| ATOM | 1529 | O | LEU | 11 | 87.769 | 8.943 | 24.365 | 1.00 | 37.61 | H | O |
| ATOM | 1530 | N | VAL | 12 | 87.961 | 8.550 | 22.165 | 1.00 | 31.23 | H | N |
| ATOM | 1531 | CA | VAL | 12 | 87.048 | 9.624 | 21.792 | 1.00 | 31.23 | H | C |
| ATOM | 1532 | CB | VAL | 12 | 87.794 | 10.800 | 21.144 | 1.00 | 52.64 | H | C |
| ATOM | 1533 | CG1 | VAL | 12 | 88.609 | 11.532 | 22.192 | 1.00 | 52.64 | H | C |

Fig. 19: A-22

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1534 | CG2 | VAL | 12 | 88.699 | 10.290 | 20.039 | 1.00 | 52.64 | H | C |
| ATOM | 1535 | C | VAL | 12 | 86.062 | 9.045 | 20.794 | 1.00 | 31.23 | H | C |
| ATOM | 1536 | O | VAL | 12 | 86.365 | 8.057 | 20.138 | 1.00 | 31.23 | H | O |
| ATOM | 1537 | N | GLN | 13 | 84.882 | 9.640 | 20.681 | 1.00 | 27.32 | H | N |
| ATOM | 1538 | CA | GLN | 13 | 83.894 | 9.126 | 19.741 | 1.00 | 27.32 | H | C |
| ATOM | 1539 | CB | GLN | 13 | 82.493 | 9.391 | 20.270 | 1.00 | 92.40 | H | C |
| ATOM | 1540 | CG | GLN | 13 | 82.206 | 8.652 | 21.553 | 1.00 | 92.40 | H | C |
| ATOM | 1541 | CD | GLN | 13 | 80.808 | 8.906 | 22.056 | 1.00 | 92.40 | H | C |
| ATOM | 1542 | OE1 | GLN | 13 | 79.836 | 8.766 | 21.310 | 1.00 | 92.40 | H | O |
| ATOM | 1543 | NE2 | GLN | 13 | 80.693 | 9.276 | 23.329 | 1.00 | 92.40 | H | N |
| ATOM | 1544 | C | GLN | 13 | 84.063 | 9.747 | 18.356 | 1.00 | 27.32 | H | C |
| ATOM | 1545 | O | GLN | 13 | 84.400 | 10.924 | 18.227 | 1.00 | 27.32 | H | O |
| ATOM | 1546 | N | PRO | 14 | 83.834 | 8.955 | 17.298 | 1.00 | 39.48 | H | N |
| ATOM | 1547 | CD | PRO | 14 | 83.418 | 7.539 | 17.302 | 1.00 | 31.44 | H | C |
| ATOM | 1548 | CA | PRO | 14 | 83.971 | 9.452 | 15.929 | 1.00 | 39.48 | H | C |
| ATOM | 1549 | CB | PRO | 14 | 83.219 | 8.406 | 15.118 | 1.00 | 31.44 | H | C |
| ATOM | 1550 | CG | PRO | 14 | 83.584 | 7.145 | 15.837 | 1.00 | 31.44 | H | C |
| ATOM | 1551 | C | PRO | 14 | 83.401 | 10.849 | 15.766 | 1.00 | 39.48 | H | C |
| ATOM | 1552 | O | PRO | 14 | 82.235 | 11.076 | 16.053 | 1.00 | 39.48 | H | O |
| ATOM | 1553 | N | GLY | 15 | 84.233 | 11.784 | 15.319 | 1.00 | 28.44 | H | N |
| ATOM | 1554 | CA | GLY | 15 | 83.788 | 13.154 | 15.130 | 1.00 | 28.44 | H | C |
| ATOM | 1555 | C | GLY | 15 | 84.048 | 14.065 | 16.323 | 1.00 | 28.44 | H | C |
| ATOM | 1556 | O | GLY | 15 | 83.759 | 15.265 | 16.269 | 1.00 | 28.44 | H | O |
| ATOM | 1557 | N | GLY | 16 | 84.588 | 13.496 | 17.401 | 1.00 | 22.09 | H | N |
| ATOM | 1558 | CA | GLY | 16 | 84.880 | 14.266 | 18.601 | 1.00 | 22.09 | H | C |
| ATOM | 1559 | C | GLY | 16 | 86.286 | 14.826 | 18.571 | 1.00 | 22.09 | H | C |
| ATOM | 1560 | O | GLY | 16 | 86.900 | 14.912 | 17.507 | 1.00 | 22.09 | H | O |
| ATOM | 1561 | N | SER | 17 | 86.819 | 15.202 | 19.726 | 1.00 | 31.69 | H | N |
| ATOM | 1562 | CA | SER | 17 | 88.161 | 15.762 | 19.749 | 1.00 | 31.69 | H | C |
| ATOM | 1563 | CB | SER | 17 | 88.085 | 17.272 | 19.592 | 1.00 | 54.23 | H | C |
| ATOM | 1564 | OG | SER | 17 | 87.308 | 17.829 | 20.625 | 1.00 | 54.23 | H | O |
| ATOM | 1565 | C | SER | 17 | 88.953 | 15.416 | 21.000 | 1.00 | 31.69 | H | C |
| ATOM | 1566 | O | SER | 17 | 88.427 | 14.824 | 21.944 | 1.00 | 31.69 | H | O |
| ATOM | 1567 | N | LEU | 18 | 90.227 | 15.794 | 20.995 | 1.00 | 31.76 | H | N |
| ATOM | 1568 | CA | LEU | 18 | 91.132 | 15.515 | 22.105 | 1.00 | 31.76 | H | C |
| ATOM | 1569 | CB | LEU | 18 | 91.452 | 14.019 | 22.124 | 1.00 | 63.56 | H | C |
| ATOM | 1570 | CG | LEU | 18 | 92.462 | 13.465 | 23.124 | 1.00 | 63.56 | H | C |
| ATOM | 1571 | CD1 | LEU | 18 | 92.121 | 13.932 | 24.536 | 1.00 | 63.56 | H | C |
| ATOM | 1572 | CD2 | LEU | 18 | 92.462 | 11.942 | 23.017 | 1.00 | 63.56 | H | C |
| ATOM | 1573 | C | LEU | 18 | 92.407 | 16.334 | 21.899 | 1.00 | 31.76 | H | C |
| ATOM | 1574 | O | LEU | 18 | 92.622 | 16.884 | 20.815 | 1.00 | 31.76 | H | O |
| ATOM | 1575 | N | ARG | 19 | 93.243 | 16.443 | 22.928 | 1.00 | 39.26 | H | N |
| ATOM | 1576 | CA | ARG | 19 | 94.475 | 17.207 | 22.781 | 1.00 | 39.26 | H | C |
| ATOM | 1577 | CB | ARG | 19 | 94.303 | 18.650 | 23.258 | 1.00 | 32.50 | H | C |
| ATOM | 1578 | CG | ARG | 19 | 95.571 | 19.474 | 23.063 | 1.00 | 32.50 | H | C |
| ATOM | 1579 | CD | ARG | 19 | 95.481 | 20.862 | 23.667 | 1.00 | 32.50 | H | C |
| ATOM | 1580 | NE | ARG | 19 | 95.387 | 20.846 | 25.125 | 1.00 | 32.50 | H | N |
| ATOM | 1581 | CZ | ARG | 19 | 95.262 | 21.936 | 25.879 | 1.00 | 32.50 | H | C |
| ATOM | 1582 | NH1 | ARG | 19 | 95.220 | 23.138 | 25.322 | 1.00 | 32.50 | H | N |
| ATOM | 1583 | NH2 | ARG | 19 | 95.162 | 21.824 | 27.193 | 1.00 | 32.50 | H | N |
| ATOM | 1584 | C | ARG | 19 | 95.668 | 16.606 | 23.500 | 1.00 | 39.26 | H | C |
| ATOM | 1585 | O | ARG | 19 | 95.687 | 16.469 | 24.732 | 1.00 | 39.26 | H | O |
| ATOM | 1586 | N | LEU | 20 | 96.677 | 16.266 | 22.709 | 1.00 | 36.74 | H | N |
| ATOM | 1587 | CA | LEU | 20 | 97.896 | 15.695 | 23.241 | 1.00 | 36.74 | H | C |
| ATOM | 1588 | CB | LEU | 20 | 98.534 | 14.737 | 22.222 | 1.00 | 31.69 | H | C |
| ATOM | 1589 | CG | LEU | 20 | 97.601 | 13.846 | 21.390 | 1.00 | 31.69 | H | C |
| ATOM | 1590 | CD1 | LEU | 20 | 98.426 | 12.870 | 20.555 | 1.00 | 31.69 | H | C |
| ATOM | 1591 | CD2 | LEU | 20 | 96.659 | 13.093 | 22.292 | 1.00 | 31.69 | H | C |
| ATOM | 1592 | C | LEU | 20 | 98.854 | 16.838 | 23.533 | 1.00 | 36.74 | H | C |
| ATOM | 1593 | O | LEU | 20 | 98.866 | 17.856 | 22.840 | 1.00 | 36.74 | H | O |
| ATOM | 1594 | N | SER | 21 | 99.638 | 16.664 | 24.584 | 1.00 | 25.68 | H | N |
| ATOM | 1595 | CA | SER | 21 | 100.635 | 17.640 | 24.974 | 1.00 | 25.68 | H | C |
| ATOM | 1596 | CB | SER | 21 | 100.273 | 18.278 | 26.307 | 1.00 | 13.03 | H | C |
| ATOM | 1597 | OG | SER | 21 | 99.718 | 17.320 | 27.175 | 1.00 | 13.03 | H | O |
| ATOM | 1598 | C | SER | 21 | 101.901 | 16.838 | 25.099 | 1.00 | 25.68 | H | C |
| ATOM | 1599 | O | SER | 21 | 101.851 | 15.635 | 25.336 | 1.00 | 25.68 | H | O |
| ATOM | 1600 | N | CYS | 22 | 103.036 | 17.498 | 24.931 | 1.00 | 22.18 | H | N |
| ATOM | 1601 | CA | CYS | 22 | 104.321 | 16.822 | 25.008 | 1.00 | 22.18 | H | C |
| ATOM | 1602 | C | CYS | 22 | 105.255 | 17.765 | 25.713 | 1.00 | 22.18 | H | C |
| ATOM | 1603 | O | CYS | 22 | 105.491 | 18.863 | 25.229 | 1.00 | 22.18 | H | O |
| ATOM | 1604 | CB | CYS | 22 | 104.804 | 16.543 | 23.603 | 1.00 | 57.35 | H | C |
| ATOM | 1605 | SG | CYS | 22 | 106.473 | 15.867 | 23.383 | 1.00 | 57.35 | H | S |
| ATOM | 1606 | N | ALA | 23 | 105.769 | 17.349 | 26.867 | 1.00 | 26.87 | H | N |

# Fig. 19: A-23

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1607 | CA | ALA | 23 | 106.669 | 18.191 | 27.654 | 1.00 | 26.87 | H | C |
| ATOM | 1608 | CB | ALA | 23 | 106.470 | 17.937 | 29.141 | 1.00 | 9.84 | H | C |
| ATOM | 1609 | C | ALA | 23 | 108.125 | 17.989 | 27.284 | 1.00 | 26.87 | H | C |
| ATOM | 1610 | O | ALA | 23 | 108.683 | 16.899 | 27.437 | 1.00 | 26.87 | H | O |
| ATOM | 1611 | N | ALA | 24 | 108.738 | 19.058 | 26.800 | 1.00 | 13.29 | H | N |
| ATOM | 1612 | CA | ALA | 24 | 110.124 | 18.988 | 26.409 | 1.00 | 13.29 | H | C |
| ATOM | 1613 | CB | ALA | 24 | 110.357 | 19.851 | 25.183 | 1.00 | 45.62 | H | C |
| ATOM | 1614 | C | ALA | 24 | 111.023 | 19.432 | 27.552 | 1.00 | 13.29 | H | C |
| ATOM | 1615 | O | ALA | 24 | 110.664 | 20.304 | 28.356 | 1.00 | 13.29 | H | O |
| ATOM | 1616 | N | SER | 25 | 112.194 | 18.819 | 27.617 | 1.00 | 22.11 | H | N |
| ATOM | 1617 | CA | SER | 25 | 113.168 | 19.152 | 28.634 | 1.00 | 22.11 | H | C |
| ATOM | 1618 | CB | SER | 25 | 112.731 | 18.582 | 29.982 | 1.00 | 51.20 | H | C |
| ATOM | 1619 | OG | SER | 25 | 112.401 | 17.214 | 29.862 | 1.00 | 51.20 | H | O |
| ATOM | 1620 | C | SER | 25 | 114.526 | 18.591 | 28.232 | 1.00 | 22.11 | H | C |
| ATOM | 1621 | O | SER | 25 | 114.614 | 17.539 | 27.590 | 1.00 | 22.11 | H | O |
| ATOM | 1622 | N | GLY | 26 | 115.582 | 19.306 | 28.591 | 1.00 | 10.76 | H | N |
| ATOM | 1623 | CA | GLY | 26 | 116.914 | 18.844 | 28.263 | 1.00 | 10.76 | H | C |
| ATOM | 1624 | C | GLY | 26 | 117.553 | 19.585 | 27.107 | 1.00 | 10.76 | H | C |
| ATOM | 1625 | O | GLY | 26 | 118.728 | 19.367 | 26.809 | 1.00 | 10.76 | H | O |
| ATOM | 1626 | N | PHE | 27 | 116.794 | 20.458 | 26.448 | 1.00 | 18.08 | H | N |
| ATOM | 1627 | CA | PHE | 27 | 117.325 | 21.207 | 25.318 | 1.00 | 18.08 | H | C |
| ATOM | 1628 | CB | PHE | 27 | 117.241 | 20.373 | 24.031 | 1.00 | 16.53 | H | C |
| ATOM | 1629 | CG | PHE | 27 | 115.842 | 19.974 | 23.651 | 1.00 | 16.53 | H | C |
| ATOM | 1630 | CD1 | PHE | 27 | 115.089 | 19.140 | 24.476 | 1.00 | 16.53 | H | C |
| ATOM | 1631 | CD2 | PHE | 27 | 115.269 | 20.448 | 22.476 | 1.00 | 16.53 | H | C |
| ATOM | 1632 | CE1 | PHE | 27 | 113.770 | 18.782 | 24.137 | 1.00 | 16.53 | H | C |
| ATOM | 1633 | CE2 | PHE | 27 | 113.958 | 20.101 | 22.125 | 1.00 | 16.53 | H | C |
| ATOM | 1634 | CZ | PHE | 27 | 113.203 | 19.268 | 22.954 | 1.00 | 16.53 | H | C |
| ATOM | 1635 | C | PHE | 27 | 116.592 | 22.528 | 25.135 | 1.00 | 18.08 | H | C |
| ATOM | 1636 | O | PHE | 27 | 115.566 | 22.780 | 25.763 | 1.00 | 18.08 | H | O |
| ATOM | 1637 | N | THR | 28 | 117.139 | 23.377 | 24.276 | 1.00 | 42.88 | H | N |
| ATOM | 1638 | CA | THR | 28 | 116.544 | 24.672 | 24.017 | 1.00 | 42.88 | H | C |
| ATOM | 1639 | CB | THR | 28 | 117.575 | 25.604 | 23.381 | 1.00 | 53.65 | H | C |
| ATOM | 1640 | OG1 | THR | 28 | 118.841 | 25.399 | 24.018 | 1.00 | 53.65 | H | O |
| ATOM | 1641 | CG2 | THR | 28 | 117.168 | 27.056 | 23.561 | 1.00 | 53.65 | H | C |
| ATOM | 1642 | C | THR | 28 | 115.369 | 24.463 | 23.074 | 1.00 | 42.88 | H | C |
| ATOM | 1643 | O | THR | 28 | 115.484 | 24.666 | 21.868 | 1.00 | 42.88 | H | O |
| ATOM | 1644 | N | PHE | 29 | 114.239 | 24.051 | 23.644 | 1.00 | 29.92 | H | N |
| ATOM | 1645 | CA | PHE | 29 | 113.004 | 23.772 | 22.901 | 1.00 | 29.92 | H | C |
| ATOM | 1646 | CB | PHE | 29 | 111.855 | 23.614 | 23.906 | 1.00 | 3.95 | H | C |
| ATOM | 1647 | CG | PHE | 29 | 110.503 | 23.347 | 23.276 | 1.00 | 3.95 | H | C |
| ATOM | 1648 | CD1 | PHE | 29 | 110.208 | 22.102 | 22.696 | 1.00 | 3.95 | H | C |
| ATOM | 1649 | CD2 | PHE | 29 | 109.504 | 24.336 | 23.283 | 1.00 | 3.95 | H | C |
| ATOM | 1650 | CE1 | PHE | 29 | 108.939 | 21.852 | 22.139 | 1.00 | 3.95 | H | C |
| ATOM | 1651 | CE2 | PHE | 29 | 108.234 | 24.092 | 22.727 | 1.00 | 3.95 | H | C |
| ATOM | 1652 | CZ | PHE | 29 | 107.953 | 22.860 | 22.160 | 1.00 | 3.95 | H | C |
| ATOM | 1653 | C | PHE | 29 | 112.611 | 24.777 | 21.797 | 1.00 | 29.92 | H | C |
| ATOM | 1654 | O | PHE | 29 | 112.390 | 24.389 | 20.647 | 1.00 | 29.92 | H | O |
| ATOM | 1655 | N | SER | 30 | 112.539 | 26.058 | 22.144 | 1.00 | 32.50 | H | N |
| ATOM | 1656 | CA | SER | 30 | 112.139 | 27.105 | 21.199 | 1.00 | 32.50 | H | C |
| ATOM | 1657 | CB | SER | 30 | 112.335 | 28.473 | 21.852 | 1.00 | 67.50 | H | C |
| ATOM | 1658 | OG | SER | 30 | 113.644 | 28.591 | 22.372 | 1.00 | 67.50 | H | O |
| ATOM | 1659 | C | SER | 30 | 112.799 | 27.107 | 19.812 | 1.00 | 32.50 | H | C |
| ATOM | 1660 | O | SER | 30 | 112.191 | 27.504 | 18.816 | 1.00 | 32.50 | H | O |
| ATOM | 1661 | N | ARG | 31 | 114.037 | 26.649 | 19.751 | 1.00 | 18.89 | H | N |
| ATOM | 1662 | CA | ARG | 31 | 114.801 | 26.636 | 18.515 | 1.00 | 18.89 | H | C |
| ATOM | 1663 | CB | ARG | 31 | 116.292 | 26.604 | 18.886 | 1.00 | 48.17 | H | C |
| ATOM | 1664 | CG | ARG | 31 | 117.217 | 25.955 | 17.887 | 1.00 | 48.17 | H | C |
| ATOM | 1665 | CD | ARG | 31 | 118.650 | 26.425 | 18.112 | 1.00 | 48.17 | H | C |
| ATOM | 1666 | NE | ARG | 31 | 119.135 | 26.203 | 19.476 | 1.00 | 48.17 | H | N |
| ATOM | 1667 | CZ | ARG | 31 | 120.228 | 26.777 | 19.980 | 1.00 | 48.17 | H | C |
| ATOM | 1668 | NH1 | ARG | 31 | 120.950 | 27.608 | 19.238 | 1.00 | 48.17 | H | N |
| ATOM | 1669 | NH2 | ARG | 31 | 120.604 | 26.524 | 21.226 | 1.00 | 48.17 | H | N |
| ATOM | 1670 | C | ARG | 31 | 114.463 | 25.523 | 17.521 | 1.00 | 18.89 | H | C |
| ATOM | 1671 | O | ARG | 31 | 114.520 | 25.723 | 16.313 | 1.00 | 18.89 | H | O |
| ATOM | 1672 | N | TYR | 32 | 114.095 | 24.353 | 18.027 | 1.00 | 15.47 | H | N |
| ATOM | 1673 | CA | TYR | 32 | 113.791 | 23.200 | 17.179 | 1.00 | 15.47 | H | C |
| ATOM | 1674 | CB | TYR | 32 | 113.949 | 21.922 | 17.996 | 1.00 | 6.03 | H | C |
| ATOM | 1675 | CG | TYR | 32 | 115.367 | 21.653 | 18.426 | 1.00 | 6.03 | H | C |
| ATOM | 1676 | CD1 | TYR | 32 | 115.934 | 22.336 | 19.500 | 1.00 | 6.03 | H | C |
| ATOM | 1677 | CE1 | TYR | 32 | 117.249 | 22.097 | 19.889 | 1.00 | 6.03 | H | C |
| ATOM | 1678 | CD2 | TYR | 32 | 116.153 | 20.722 | 17.747 | 1.00 | 6.03 | H | C |
| ATOM | 1679 | CE2 | TYR | 32 | 117.467 | 20.477 | 18.122 | 1.00 | 6.03 | H | C |

Fig. 19: A-24

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1680 | CZ | TYR | 32 | 118.013 | 21.165 | 19.198 | 1.00 | 6.03 | H | C |
| ATOM | 1681 | OH | TYR | 32 | 119.317 | 20.907 | 19.597 | 1.00 | 6.03 | H | O |
| ATOM | 1682 | C | TYR | 32 | 112.426 | 23.184 | 16.534 | 1.00 | 15.47 | H | C |
| ATOM | 1683 | O | TYR | 32 | 111.480 | 23.748 | 17.058 | 1.00 | 15.47 | H | O |
| ATOM | 1684 | N | THR | 33 | 112.309 | 22.545 | 15.382 | 1.00 | 10.91 | H | N |
| ATOM | 1685 | CA | THR | 33 | 110.988 | 22.451 | 14.792 | 1.00 | 10.91 | H | C |
| ATOM | 1686 | CB | THR | 33 | 111.032 | 22.556 | 13.230 | 1.00 | 11.96 | H | C |
| ATOM | 1687 | OG1 | THR | 33 | 111.079 | 21.259 | 12.639 | 1.00 | 11.96 | H | O |
| ATOM | 1688 | CG2 | THR | 33 | 112.251 | 23.338 | 12.786 | 1.00 | 11.96 | H | C |
| ATOM | 1689 | C | THR | 33 | 110.501 | 21.082 | 15.303 | 1.00 | 10.91 | H | C |
| ATOM | 1690 | O | THR | 33 | 111.188 | 20.061 | 15.157 | 1.00 | 10.91 | H | O |
| ATOM | 1691 | N | MET | 34 | 109.348 | 21.070 | 15.960 | 1.00 | 21.14 | H | N |
| ATOM | 1692 | CA | MET | 34 | 108.815 | 19.835 | 16.518 | 1.00 | 21.14 | H | C |
| ATOM | 1693 | CB | MET | 34 | 108.188 | 20.094 | 17.888 | 1.00 | 16.88 | H | C |
| ATOM | 1694 | CG | MET | 34 | 109.035 | 20.899 | 18.847 | 1.00 | 16.88 | H | C |
| ATOM | 1695 | SD | MET | 34 | 110.603 | 20.131 | 19.122 | 1.00 | 16.88 | H | S |
| ATOM | 1696 | CE | MET | 34 | 110.155 | 18.770 | 20.240 | 1.00 | 16.88 | H | C |
| ATOM | 1697 | C | MET | 34 | 107.760 | 19.218 | 15.614 | 1.00 | 21.14 | H | C |
| ATOM | 1698 | O | MET | 34 | 107.160 | 19.905 | 14.781 | 1.00 | 21.14 | H | O |
| ATOM | 1699 | N | SER | 35 | 107.519 | 17.925 | 15.802 | 1.00 | 15.88 | H | N |
| ATOM | 1700 | CA | SER | 35 | 106.533 | 17.232 | 14.997 | 1.00 | 15.88 | H | C |
| ATOM | 1701 | CB | SER | 35 | 107.205 | 16.581 | 13.794 | 1.00 | 13.53 | H | C |
| ATOM | 1702 | OG | SER | 35 | 107.895 | 17.550 | 13.034 | 1.00 | 13.53 | H | O |
| ATOM | 1703 | C | SER | 35 | 105.767 | 16.168 | 15.763 | 1.00 | 15.88 | H | C |
| ATOM | 1704 | O | SER | 35 | 106.058 | 15.867 | 16.926 | 1.00 | 15.88 | H | O |
| ATOM | 1705 | N | TRP | 36 | 104.765 | 15.617 | 15.087 | 1.00 | 13.73 | H | N |
| ATOM | 1706 | CA | TRP | 36 | 103.948 | 14.556 | 15.626 | 1.00 | 13.73 | H | C |
| ATOM | 1707 | CB | TRP | 36 | 102.510 | 15.023 | 15.849 | 1.00 | 20.04 | H | C |
| ATOM | 1708 | CG | TRP | 36 | 102.337 | 15.903 | 17.039 | 1.00 | 20.04 | H | C |
| ATOM | 1709 | CD2 | TRP | 36 | 102.259 | 15.489 | 18.406 | 1.00 | 20.04 | H | C |
| ATOM | 1710 | CE2 | TRP | 36 | 102.112 | 16.654 | 19.186 | 1.00 | 20.04 | H | C |
| ATOM | 1711 | CE3 | TRP | 36 | 102.301 | 14.248 | 19.046 | 1.00 | 20.04 | H | C |
| ATOM | 1712 | CD1 | TRP | 36 | 102.236 | 17.255 | 17.045 | 1.00 | 20.04 | H | C |
| ATOM | 1713 | NE1 | TRP | 36 | 102.100 | 17.716 | 18.329 | 1.00 | 20.04 | H | N |
| ATOM | 1714 | CZ2 | TRP | 36 | 102.004 | 16.622 | 20.576 | 1.00 | 20.04 | H | C |
| ATOM | 1715 | CZ3 | TRP | 36 | 102.192 | 14.211 | 20.442 | 1.00 | 20.04 | H | C |
| ATOM | 1716 | CH2 | TRP | 36 | 102.044 | 15.396 | 21.190 | 1.00 | 20.04 | H | C |
| ATOM | 1717 | C | TRP | 36 | 103.978 | 13.470 | 14.565 | 1.00 | 13.73 | H | C |
| ATOM | 1718 | O | TRP | 36 | 103.879 | 13.769 | 13.373 | 1.00 | 13.73 | H | O |
| ATOM | 1719 | N | VAL | 37 | 104.138 | 12.221 | 15.006 | 1.00 | 21.09 | H | N |
| ATOM | 1720 | CA | VAL | 37 | 104.179 | 11.054 | 14.125 | 1.00 | 21.09 | H | C |
| ATOM | 1721 | CB | VAL | 37 | 105.622 | 10.464 | 14.053 | 1.00 | 6.36 | H | C |
| ATOM | 1722 | CG1 | VAL | 37 | 105.591 | 9.017 | 13.642 | 1.00 | 6.36 | H | C |
| ATOM | 1723 | CG2 | VAL | 37 | 106.461 | 11.253 | 13.057 | 1.00 | 6.36 | H | C |
| ATOM | 1724 | C | VAL | 37 | 103.229 | 10.041 | 14.748 | 1.00 | 21.09 | H | C |
| ATOM | 1725 | O | VAL | 37 | 103.144 | 9.940 | 15.963 | 1.00 | 21.09 | H | O |
| ATOM | 1726 | N | ARG | 38 | 102.508 | 9.294 | 13.929 | 1.00 | 17.98 | H | N |
| ATOM | 1727 | CA | ARG | 38 | 101.562 | 8.309 | 14.454 | 1.00 | 17.98 | H | C |
| ATOM | 1728 | CB | ARG | 38 | 100.133 | 8.697 | 14.058 | 1.00 | 13.99 | H | C |
| ATOM | 1729 | CG | ARG | 38 | 100.106 | 9.210 | 12.633 | 1.00 | 13.99 | H | C |
| ATOM | 1730 | CD | ARG | 38 | 98.899 | 8.817 | 11.839 | 1.00 | 13.99 | H | C |
| ATOM | 1731 | NE | ARG | 38 | 97.664 | 9.434 | 12.289 | 1.00 | 13.99 | H | N |
| ATOM | 1732 | CZ | ARG | 38 | 96.652 | 9.707 | 11.470 | 1.00 | 13.99 | H | C |
| ATOM | 1733 | NH1 | ARG | 38 | 96.744 | 9.432 | 10.171 | 1.00 | 13.99 | H | N |
| ATOM | 1734 | NH2 | ARG | 38 | 95.533 | 10.224 | 11.960 | 1.00 | 13.99 | H | N |
| ATOM | 1735 | C | ARG | 38 | 101.856 | 6.925 | 13.895 | 1.00 | 17.98 | H | C |
| ATOM | 1736 | O | ARG | 38 | 102.468 | 6.785 | 12.840 | 1.00 | 17.98 | H | O |
| ATOM | 1737 | N | GLN | 39 | 101.386 | 5.909 | 14.604 | 1.00 | 17.63 | H | N |
| ATOM | 1738 | CA | GLN | 39 | 101.560 | 4.521 | 14.200 | 1.00 | 17.63 | H | C |
| ATOM | 1739 | CB | GLN | 39 | 102.659 | 3.866 | 15.051 | 1.00 | 12.11 | H | C |
| ATOM | 1740 | CG | GLN | 39 | 102.976 | 2.424 | 14.712 | 1.00 | 12.11 | H | C |
| ATOM | 1741 | CD | GLN | 39 | 104.396 | 2.025 | 15.134 | 1.00 | 12.11 | H | C |
| ATOM | 1742 | OE1 | GLN | 39 | 104.811 | 2.262 | 16.272 | 1.00 | 12.11 | H | O |
| ATOM | 1743 | NE2 | GLN | 39 | 105.143 | 1.414 | 14.212 | 1.00 | 12.11 | H | N |
| ATOM | 1744 | C | GLN | 39 | 100.206 | 3.847 | 14.429 | 1.00 | 17.63 | H | C |
| ATOM | 1745 | O | GLN | 39 | 99.712 | 3.770 | 15.562 | 1.00 | 17.63 | H | O |
| ATOM | 1746 | N | ALA | 40 | 99.590 | 3.399 | 13.344 | 1.00 | 55.11 | H | N |
| ATOM | 1747 | CA | ALA | 40 | 98.300 | 2.737 | 13.436 | 1.00 | 55.11 | H | C |
| ATOM | 1748 | CB | ALA | 40 | 97.605 | 2.754 | 12.088 | 1.00 | 43.12 | H | C |
| ATOM | 1749 | C | ALA | 40 | 98.536 | 1.302 | 13.881 | 1.00 | 55.11 | H | C |
| ATOM | 1750 | O | ALA | 40 | 99.626 | 0.762 | 13.687 | 1.00 | 55.11 | H | O |
| ATOM | 1751 | N | PRO | 41 | 97.517 | 0.670 | 14.491 | 1.00 | 55.83 | H | N |
| ATOM | 1752 | CD | PRO | 41 | 96.189 | 1.237 | 14.782 | 1.00 | 86.02 | H | C |

Fig. 19: A-25

```
ATOM   1753  CA  PRO  41      97.600  -0.712  14.969  1.00  55.83  H  C
ATOM   1754  CB  PRO  41      96.169  -1.009  15.400  1.00  86.02  H  C
ATOM   1755  CG  PRO  41      95.681   0.315  15.859  1.00  86.02  H  C
ATOM   1756  C   PRO  41      98.057  -1.624  13.838  1.00  55.83  H  C
ATOM   1757  O   PRO  41      97.423  -1.670  12.781  1.00  55.83  H  O
ATOM   1758  N   GLY  42      99.160  -2.335  14.061  1.00  43.01  H  N
ATOM   1759  CA  GLY  42      99.684  -3.227  13.042  1.00  43.01  H  C
ATOM   1760  C   GLY  42     100.227  -2.529  11.800  1.00  43.01  H  C
ATOM   1761  O   GLY  42     100.480  -3.175  10.775  1.00  43.01  H  O
ATOM   1762  N   LYS  43     100.415  -1.212  11.882  1.00  46.16  H  N
ATOM   1763  CA  LYS  43     100.922  -0.446  10.750  1.00  46.16  H  C
ATOM   1764  CB  LYS  43      99.896   0.612  10.334  1.00  59.60  H  C
ATOM   1765  CG  LYS  43      98.800   0.081   9.421  1.00  59.60  H  C
ATOM   1766  CD  LYS  43      98.003  -1.023  10.079  1.00  59.60  H  C
ATOM   1767  CE  LYS  43      97.230  -1.831   9.047  1.00  59.60  H  C
ATOM   1768  NZ  LYS  43      98.125  -2.590   8.124  1.00  59.60  H  N
ATOM   1769  C   LYS  43     102.278   0.215  10.994  1.00  46.16  H  C
ATOM   1770  O   LYS  43     102.889   0.060  12.063  1.00  46.16  H  O
ATOM   1771  N   GLY  44     102.742   0.942   9.976  1.00  50.42  H  N
ATOM   1772  CA  GLY  44     104.016   1.631  10.054  1.00  50.42  H  C
ATOM   1773  C   GLY  44     103.916   3.004  10.691  1.00  50.42  H  C
ATOM   1774  O   GLY  44     103.001   3.281  11.462  1.00  50.42  H  O
ATOM   1775  N   LEU  45     104.862   3.870  10.347  1.00  25.59  H  N
ATOM   1776  CA  LEU  45     104.933   5.229  10.883  1.00  25.59  H  C
ATOM   1777  CB  LEU  45     106.387   5.544  11.224  1.00   8.94  H  C
ATOM   1778  CG  LEU  45     107.011   4.480  12.118  1.00   8.94  H  C
ATOM   1779  CD1 LEU  45     108.520   4.578  12.054  1.00   8.94  H  C
ATOM   1780  CD2 LEU  45     106.481   4.638  13.541  1.00   8.94  H  C
ATOM   1781  C   LEU  45     104.394   6.259   9.893  1.00  25.59  H  C
ATOM   1782  O   LEU  45     104.613   6.142   8.684  1.00  25.59  H  O
ATOM   1783  N   GLU  46     103.698   7.268  10.411  1.00  28.67  H  N
ATOM   1784  CA  GLU  46     103.111   8.308   9.569  1.00  28.67  H  C
ATOM   1785  CB  GLU  46     101.617   8.045   9.370  1.00  21.38  H  C
ATOM   1786  CG  GLU  46     100.977   8.902   8.304  1.00  21.38  H  C
ATOM   1787  CD  GLU  46      99.555   8.471   7.972  1.00  21.38  H  C
ATOM   1788  OE1 GLU  46      98.711   8.399   8.903  1.00  21.38  H  O
ATOM   1789  OE2 GLU  46      99.283   8.214   6.776  1.00  21.38  H  O
ATOM   1790  C   GLU  46     103.304   9.698  10.152  1.00  28.67  H  C
ATOM   1791  O   GLU  46     102.942   9.962  11.301  1.00  28.67  H  O
ATOM   1792  N   TRP  47     103.887  10.579   9.347  1.00   2.61  H  N
ATOM   1793  CA  TRP  47     104.132  11.944   9.758  1.00   2.61  H  C
ATOM   1794  CB  TRP  47     105.055  12.618   8.757  1.00  14.19  H  C
ATOM   1795  CG  TRP  47     105.068  14.095   8.904  1.00  14.19  H  C
ATOM   1796  CD2 TRP  47     104.446  15.035   8.036  1.00  14.19  H  C
ATOM   1797  CE2 TRP  47     104.681  16.323   8.578  1.00  14.19  H  C
ATOM   1798  CE3 TRP  47     103.709  14.919   6.852  1.00  14.19  H  C
ATOM   1799  CD1 TRP  47     105.644  14.824   9.914  1.00  14.19  H  C
ATOM   1800  NE1 TRP  47     105.418  16.161   9.723  1.00  14.19  H  N
ATOM   1801  CZ2 TRP  47     104.201  17.490   7.969  1.00  14.19  H  C
ATOM   1802  CZ3 TRP  47     103.233  16.074   6.248  1.00  14.19  H  C
ATOM   1803  CH2 TRP  47     103.480  17.344   6.808  1.00  14.19  H  C
ATOM   1804  C   TRP  47     102.791  12.673   9.802  1.00   2.61  H  C
ATOM   1805  O   TRP  47     102.083  12.752   8.796  1.00   2.61  H  O
ATOM   1806  N   VAL  48     102.443  13.215  10.962  1.00  34.26  H  N
ATOM   1807  CA  VAL  48     101.165  13.895  11.114  1.00  34.26  H  C
ATOM   1808  CB  VAL  48     100.576  13.639  12.523  1.00  16.29  H  C
ATOM   1809  CG1 VAL  48      99.137  14.148  12.623  1.00  16.29  H  C
ATOM   1810  CG2 VAL  48     100.624  12.187  12.812  1.00  16.29  H  C
ATOM   1811  C   VAL  48     101.246  15.393  10.884  1.00  34.26  H  C
ATOM   1812  O   VAL  48     100.563  15.932  10.015  1.00  34.26  H  O
ATOM   1813  N   ALA  49     102.078  16.068  11.665  1.00  19.79  H  N
ATOM   1814  CA  ALA  49     102.198  17.505  11.533  1.00  19.79  H  C
ATOM   1815  CB  ALA  49     101.052  18.193  12.288  1.00   1.87  H  C
ATOM   1816  C   ALA  49     103.542  17.994  12.041  1.00  19.79  H  C
ATOM   1817  O   ALA  49     104.295  17.244  12.645  1.00  19.79  H  O
ATOM   1818  N   THR  50     103.816  19.271  11.795  1.00  29.76  H  N
ATOM   1819  CA  THR  50     105.067  19.906  12.184  1.00  29.76  H  C
ATOM   1820  CB  THR  50     106.142  19.637  11.127  1.00  20.69  H  C
ATOM   1821  OG1 THR  50     106.390  18.232  11.065  1.00  20.69  H  O
ATOM   1822  CG2 THR  50     107.422  20.357  11.460  1.00  20.69  H  C
ATOM   1823  C   THR  50     104.897  21.416  12.327  1.00  29.76  H  C
ATOM   1824  O   THR  50     104.113  22.035  11.616  1.00  29.76  H  O
ATOM   1825  N   ILE  51     105.649  21.994  13.258  1.00  20.54  H  N
```

Fig. 19: A-26

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1826 | CA | ILE | 51 | 105.626 | 23.424 | 13.530 | 1.00 | 20.54 | H | C |
| ATOM | 1827 | CB | ILE | 51 | 104.824 | 23.714 | 14.816 | 1.00 | 27.11 | H | C |
| ATOM | 1828 | CG2 | ILE | 51 | 105.430 | 22.955 | 15.975 | 1.00 | 27.11 | H | C |
| ATOM | 1829 | CG1 | ILE | 51 | 104.805 | 25.217 | 15.108 | 1.00 | 27.11 | H | C |
| ATOM | 1830 | CD1 | ILE | 51 | 104.073 | 25.593 | 16.389 | 1.00 | 27.11 | H | C |
| ATOM | 1831 | C | ILE | 51 | 107.090 | 23.813 | 13.723 | 1.00 | 20.54 | H | C |
| ATOM | 1832 | O | ILE | 51 | 107.781 | 23.208 | 14.533 | 1.00 | 20.54 | H | O |
| ATOM | 1833 | N | SER | 52 | 107.565 | 24.803 | 12.970 | 1.00 | 28.49 | H | N |
| ATOM | 1834 | CA | SER | 52 | 108.962 | 25.234 | 13.047 | 1.00 | 28.49 | H | C |
| ATOM | 1835 | CB | SER | 52 | 109.356 | 26.018 | 11.797 | 1.00 | 35.37 | H | C |
| ATOM | 1836 | OG | SER | 52 | 108.819 | 27.332 | 11.832 | 1.00 | 35.37 | H | O |
| ATOM | 1837 | C | SER | 52 | 109.236 | 26.105 | 14.256 | 1.00 | 28.49 | H | C |
| ATOM | 1838 | O | SER | 52 | 108.316 | 26.461 | 14.994 | 1.00 | 28.49 | H | O |
| ATOM | 1839 | N | GLY | 53 | 110.509 | 26.452 | 14.451 | 1.00 | 16.74 | H | N |
| ATOM | 1840 | CA | GLY | 53 | 110.864 | 27.295 | 15.568 | 1.00 | 16.74 | H | C |
| ATOM | 1841 | C | GLY | 53 | 110.203 | 28.651 | 15.410 | 1.00 | 16.74 | H | C |
| ATOM | 1842 | O | GLY | 53 | 110.093 | 29.412 | 16.369 | 1.00 | 16.74 | H | O |
| ATOM | 1843 | N | GLY | 54 | 109.746 | 28.939 | 14.192 | 1.00 | 26.55 | H | N |
| ATOM | 1844 | CA | GLY | 54 | 109.120 | 30.218 | 13.907 | 1.00 | 26.55 | H | C |
| ATOM | 1845 | C | GLY | 54 | 107.605 | 30.253 | 13.815 | 1.00 | 26.55 | H | C |
| ATOM | 1846 | O | GLY | 54 | 107.020 | 31.317 | 13.607 | 1.00 | 26.55 | H | O |
| ATOM | 1847 | N | GLY | 55 | 106.953 | 29.105 | 13.948 | 1.00 | 34.83 | H | N |
| ATOM | 1848 | CA | GLY | 55 | 105.505 | 29.105 | 13.889 | 1.00 | 34.83 | H | C |
| ATOM | 1849 | C | GLY | 55 | 104.878 | 28.610 | 12.604 | 1.00 | 34.83 | H | C |
| ATOM | 1850 | O | GLY | 55 | 103.657 | 28.663 | 12.458 | 1.00 | 34.83 | H | O |
| ATOM | 1851 | N | HIS | 56 | 105.683 | 28.149 | 11.655 | 1.00 | 20.17 | H | N |
| ATOM | 1852 | CA | HIS | 56 | 105.091 | 27.643 | 10.426 | 1.00 | 20.17 | H | C |
| ATOM | 1853 | CB | HIS | 56 | 106.117 | 27.522 | 9.302 | 1.00 | 75.35 | H | C |
| ATOM | 1854 | CG | HIS | 56 | 106.829 | 28.797 | 8.996 | 1.00 | 75.35 | H | C |
| ATOM | 1855 | CD2 | HIS | 56 | 106.561 | 29.773 | 8.096 | 1.00 | 75.35 | H | C |
| ATOM | 1856 | ND1 | HIS | 56 | 107.959 | 29.201 | 9.677 | 1.00 | 75.35 | H | N |
| ATOM | 1857 | CE1 | HIS | 56 | 108.356 | 30.370 | 9.209 | 1.00 | 75.35 | H | C |
| ATOM | 1858 | NE2 | HIS | 56 | 107.525 | 30.739 | 8.250 | 1.00 | 75.35 | H | N |
| ATOM | 1859 | C | HIS | 56 | 104.585 | 26.266 | 10.774 | 1.00 | 20.17 | H | C |
| ATOM | 1860 | O | HIS | 56 | 105.309 | 25.465 | 11.350 | 1.00 | 20.17 | H | O |
| ATOM | 1861 | N | THR | 57 | 103.331 | 25.994 | 10.458 | 1.00 | 9.30 | H | N |
| ATOM | 1862 | CA | THR | 57 | 102.793 | 24.676 | 10.728 | 1.00 | 9.30 | H | C |
| ATOM | 1863 | CB | THR | 57 | 101.437 | 24.766 | 11.475 | 1.00 | 25.93 | H | C |
| ATOM | 1864 | OG1 | THR | 57 | 100.483 | 25.493 | 10.691 | 1.00 | 25.93 | H | O |
| ATOM | 1865 | CG2 | THR | 57 | 101.624 | 25.460 | 12.821 | 1.00 | 25.93 | H | C |
| ATOM | 1866 | C | THR | 57 | 102.657 | 23.911 | 9.403 | 1.00 | 9.30 | H | C |
| ATOM | 1867 | O | THR | 57 | 102.437 | 24.503 | 8.348 | 1.00 | 9.30 | H | O |
| ATOM | 1868 | N | TYR | 58 | 102.849 | 22.598 | 9.463 | 1.00 | 10.35 | H | N |
| ATOM | 1869 | CA | TYR | 58 | 102.739 | 21.729 | 8.293 | 1.00 | 10.35 | H | C |
| ATOM | 1870 | CB | TYR | 58 | 104.115 | 21.217 | 7.912 | 1.00 | 22.31 | H | C |
| ATOM | 1871 | CG | TYR | 58 | 105.023 | 22.324 | 7.485 | 1.00 | 22.31 | H | C |
| ATOM | 1872 | CD1 | TYR | 58 | 105.051 | 22.744 | 6.167 | 1.00 | 22.31 | H | C |
| ATOM | 1873 | CE1 | TYR | 58 | 105.871 | 23.765 | 5.768 | 1.00 | 22.31 | H | C |
| ATOM | 1874 | CD2 | TYR | 58 | 105.843 | 22.967 | 8.399 | 1.00 | 22.31 | H | C |
| ATOM | 1875 | CE2 | TYR | 58 | 106.667 | 23.997 | 8.007 | 1.00 | 22.31 | H | C |
| ATOM | 1876 | CZ | TYR | 58 | 106.674 | 24.388 | 6.689 | 1.00 | 22.31 | H | C |
| ATOM | 1877 | OH | TYR | 58 | 107.478 | 25.419 | 6.279 | 1.00 | 22.31 | H | O |
| ATOM | 1878 | C | TYR | 58 | 101.812 | 20.565 | 8.635 | 1.00 | 10.35 | H | C |
| ATOM | 1879 | O | TYR | 58 | 101.699 | 20.164 | 9.801 | 1.00 | 10.35 | H | O |
| ATOM | 1880 | N | TYR | 59 | 101.147 | 20.007 | 7.634 | 1.00 | 15.64 | H | N |
| ATOM | 1881 | CA | TYR | 59 | 100.219 | 18.936 | 7.931 | 1.00 | 15.64 | H | C |
| ATOM | 1882 | CB | TYR | 59 | 98.843 | 19.542 | 8.203 | 1.00 | 11.32 | H | C |
| ATOM | 1883 | CG | TYR | 59 | 98.803 | 20.511 | 9.360 | 1.00 | 11.32 | H | C |
| ATOM | 1884 | CD1 | TYR | 59 | 98.625 | 20.058 | 10.661 | 1.00 | 11.32 | H | C |
| ATOM | 1885 | CE1 | TYR | 59 | 98.540 | 20.942 | 11.731 | 1.00 | 11.32 | H | C |
| ATOM | 1886 | CD2 | TYR | 59 | 98.912 | 21.886 | 9.148 | 1.00 | 11.32 | H | C |
| ATOM | 1887 | CE2 | TYR | 59 | 98.835 | 22.783 | 10.208 | 1.00 | 11.32 | H | C |
| ATOM | 1888 | CZ | TYR | 59 | 98.640 | 22.302 | 11.502 | 1.00 | 11.32 | H | C |
| ATOM | 1889 | OH | TYR | 59 | 98.498 | 23.177 | 12.557 | 1.00 | 11.32 | H | O |
| ATOM | 1890 | C | TYR | 59 | 100.071 | 17.883 | 6.856 | 1.00 | 15.64 | H | C |
| ATOM | 1891 | O | TYR | 59 | 100.150 | 18.182 | 5.666 | 1.00 | 15.64 | H | O |
| ATOM | 1892 | N | LEU | 60 | 99.854 | 16.644 | 7.286 | 1.00 | 33.81 | H | N |
| ATOM | 1893 | CA | LEU | 60 | 99.616 | 15.539 | 6.366 | 1.00 | 33.81 | H | C |
| ATOM | 1894 | CB | LEU | 60 | 99.625 | 14.217 | 7.135 | 1.00 | 13.27 | H | C |
| ATOM | 1895 | CG | LEU | 60 | 99.371 | 12.896 | 6.406 | 1.00 | 13.27 | H | C |
| ATOM | 1896 | CD1 | LEU | 60 | 100.681 | 12.371 | 5.800 | 1.00 | 13.27 | H | C |
| ATOM | 1897 | CD2 | LEU | 60 | 98.804 | 11.882 | 7.397 | 1.00 | 13.27 | H | C |
| ATOM | 1898 | C | LEU | 60 | 98.198 | 15.861 | 5.869 | 1.00 | 33.81 | H | C |

Fig. 19: A-27

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1899 | O | LEU | 60 | 97.329 | 16.255 | 6.659 | 1.00 | 33.81 | H | O |
| ATOM | 1900 | N | ASP | 61 | 97.962 | 15.710 | 4.573 | 1.00 | 24.56 | H | N |
| ATOM | 1901 | CA | ASP | 61 | 96.659 | 16.028 | 3.991 | 1.00 | 24.56 | H | C |
| ATOM | 1902 | CB | ASP | 61 | 96.639 | 15.579 | 2.530 | 1.00 | 55.35 | H | C |
| ATOM | 1903 | CG | ASP | 61 | 97.719 | 16.260 | 1.708 | 1.00 | 55.35 | H | C |
| ATOM | 1904 | OD1 | ASP | 61 | 98.919 | 16.083 | 2.023 | 1.00 | 55.35 | H | O |
| ATOM | 1905 | OD2 | ASP | 61 | 97.374 | 16.981 | 0.754 | 1.00 | 55.35 | H | O |
| ATOM | 1906 | C | ASP | 61 | 95.436 | 15.495 | 4.731 | 1.00 | 24.56 | H | C |
| ATOM | 1907 | O | ASP | 61 | 94.515 | 16.254 | 5.043 | 1.00 | 24.56 | H | O |
| ATOM | 1908 | N | SER | 62 | 95.432 | 14.198 | 5.024 | 1.00 | 20.78 | H | N |
| ATOM | 1909 | CA | SER | 62 | 94.317 | 13.567 | 5.717 | 1.00 | 20.78 | H | C |
| ATOM | 1910 | CB | SER | 62 | 94.630 | 12.085 | 5.955 | 1.00 | 31.68 | H | C |
| ATOM | 1911 | OG | SER | 62 | 95.820 | 11.902 | 6.708 | 1.00 | 31.68 | H | O |
| ATOM | 1912 | C | SER | 62 | 93.882 | 14.216 | 7.044 | 1.00 | 20.78 | H | C |
| ATOM | 1913 | O | SER | 62 | 92.732 | 14.053 | 7.475 | 1.00 | 20.78 | H | O |
| ATOM | 1914 | N | VAL | 63 | 94.779 | 14.949 | 7.695 | 1.00 | 24.27 | H | N |
| ATOM | 1915 | CA | VAL | 63 | 94.439 | 15.567 | 8.968 | 1.00 | 24.27 | H | C |
| ATOM | 1916 | CB | VAL | 63 | 95.478 | 15.202 | 10.049 | 1.00 | 45.54 | H | C |
| ATOM | 1917 | CG1 | VAL | 63 | 95.642 | 13.698 | 10.110 | 1.00 | 45.54 | H | C |
| ATOM | 1918 | CG2 | VAL | 63 | 96.812 | 15.873 | 9.752 | 1.00 | 45.54 | H | C |
| ATOM | 1919 | C | VAL | 63 | 94.374 | 17.083 | 8.839 | 1.00 | 24.27 | H | C |
| ATOM | 1920 | O | VAL | 63 | 94.112 | 17.812 | 9.823 | 1.00 | 24.27 | H | O |
| ATOM | 1921 | N | LYS | 64 | 94.611 | 17.556 | 7.618 | 1.00 | 38.99 | H | N |
| ATOM | 1922 | CA | LYS | 64 | 94.611 | 18.985 | 7.348 | 1.00 | 38.99 | H | C |
| ATOM | 1923 | CB | LYS | 64 | 94.983 | 19.235 | 5.889 | 1.00 | 39.16 | H | C |
| ATOM | 1924 | CG | LYS | 64 | 95.736 | 20.528 | 5.671 | 1.00 | 39.16 | H | C |
| ATOM | 1925 | CD | LYS | 64 | 96.417 | 20.521 | 4.309 | 1.00 | 39.16 | H | C |
| ATOM | 1926 | CE | LYS | 64 | 97.432 | 19.380 | 4.176 | 1.00 | 39.16 | H | C |
| ATOM | 1927 | NZ | LYS | 64 | 98.011 | 19.296 | 2.803 | 1.00 | 39.16 | H | N |
| ATOM | 1928 | C | LYS | 64 | 93.262 | 19.607 | 7.667 | 1.00 | 38.99 | H | C |
| ATOM | 1929 | O | LYS | 64 | 92.240 | 19.212 | 7.121 | 1.00 | 38.99 | H | O |
| ATOM | 1930 | N | GLY | 65 | 93.263 | 20.577 | 8.567 | 1.00 | 28.42 | H | N |
| ATOM | 1931 | CA | GLY | 65 | 92.019 | 21.219 | 8.918 | 1.00 | 28.42 | H | C |
| ATOM | 1932 | C | GLY | 65 | 91.277 | 20.501 | 10.021 | 1.00 | 28.42 | H | C |
| ATOM | 1933 | O | GLY | 65 | 90.271 | 21.005 | 10.509 | 1.00 | 28.42 | H | O |
| ATOM | 1934 | N | ARG | 66 | 91.751 | 19.324 | 10.414 | 1.00 | 48.07 | H | N |
| ATOM | 1935 | CA | ARG | 66 | 91.098 | 18.588 | 11.488 | 1.00 | 48.07 | H | C |
| ATOM | 1936 | CB | ARG | 66 | 90.783 | 17.154 | 11.064 | 1.00 | 36.61 | H | C |
| ATOM | 1937 | CG | ARG | 66 | 89.845 | 17.052 | 9.887 | 1.00 | 36.61 | H | C |
| ATOM | 1938 | CD | ARG | 66 | 89.484 | 15.608 | 9.571 | 1.00 | 36.61 | H | C |
| ATOM | 1939 | NE | ARG | 66 | 90.654 | 14.750 | 9.346 | 1.00 | 36.61 | H | N |
| ATOM | 1940 | CZ | ARG | 66 | 91.133 | 13.877 | 10.236 | 1.00 | 36.61 | H | C |
| ATOM | 1941 | NH1 | ARG | 66 | 90.545 | 13.739 | 11.421 | 1.00 | 36.61 | H | N |
| ATOM | 1942 | NH2 | ARG | 66 | 92.203 | 13.144 | 9.944 | 1.00 | 36.61 | H | N |
| ATOM | 1943 | C | ARG | 66 | 92.018 | 18.568 | 12.687 | 1.00 | 48.07 | H | C |
| ATOM | 1944 | O | ARG | 66 | 91.584 | 18.312 | 13.808 | 1.00 | 48.07 | H | O |
| ATOM | 1945 | N | PHE | 67 | 93.296 | 18.839 | 12.438 | 1.00 | 31.81 | H | N |
| ATOM | 1946 | CA | PHE | 67 | 94.304 | 18.854 | 13.490 | 1.00 | 31.81 | H | C |
| ATOM | 1947 | CB | PHE | 67 | 95.372 | 17.802 | 13.211 | 1.00 | 34.94 | H | C |
| ATOM | 1948 | CG | PHE | 67 | 94.937 | 16.394 | 13.444 | 1.00 | 34.94 | H | C |
| ATOM | 1949 | CD1 | PHE | 67 | 93.763 | 15.907 | 12.902 | 1.00 | 34.94 | H | C |
| ATOM | 1950 | CD2 | PHE | 67 | 95.748 | 15.530 | 14.158 | 1.00 | 34.94 | H | C |
| ATOM | 1951 | CE1 | PHE | 67 | 93.400 | 14.564 | 13.063 | 1.00 | 34.94 | H | C |
| ATOM | 1952 | CE2 | PHE | 67 | 95.400 | 14.192 | 14.326 | 1.00 | 34.94 | H | C |
| ATOM | 1953 | CZ | PHE | 67 | 94.222 | 13.706 | 13.777 | 1.00 | 34.94 | H | C |
| ATOM | 1954 | C | PHE | 67 | 94.989 | 20.209 | 13.520 | 1.00 | 31.81 | H | C |
| ATOM | 1955 | O | PHE | 67 | 95.054 | 20.899 | 12.501 | 1.00 | 31.81 | H | O |
| ATOM | 1956 | N | THR | 68 | 95.511 | 20.587 | 14.683 | 1.00 | 27.20 | H | N |
| ATOM | 1957 | CA | THR | 68 | 96.233 | 21.851 | 14.804 | 1.00 | 27.20 | H | C |
| ATOM | 1958 | CB | THR | 68 | 95.344 | 22.998 | 15.384 | 1.00 | 14.56 | H | C |
| ATOM | 1959 | OG1 | THR | 68 | 94.400 | 23.434 | 14.399 | 1.00 | 14.56 | H | O |
| ATOM | 1960 | CG2 | THR | 68 | 96.196 | 24.192 | 15.758 | 1.00 | 14.56 | H | C |
| ATOM | 1961 | C | THR | 68 | 97.466 | 21.680 | 15.689 | 1.00 | 27.20 | H | C |
| ATOM | 1962 | O | THR | 68 | 97.355 | 21.393 | 16.882 | 1.00 | 27.20 | H | O |
| ATOM | 1963 | N | ILE | 69 | 98.643 | 21.847 | 15.099 | 1.00 | 22.74 | H | N |
| ATOM | 1964 | CA | ILE | 69 | 99.869 | 21.718 | 15.861 | 1.00 | 22.74 | H | C |
| ATOM | 1965 | CB | ILE | 69 | 100.991 | 21.084 | 15.020 | 1.00 | 13.28 | H | C |
| ATOM | 1966 | CG2 | ILE | 69 | 101.417 | 22.022 | 13.933 | 1.00 | 13.28 | H | C |
| ATOM | 1967 | CG1 | ILE | 69 | 102.188 | 20.736 | 15.908 | 1.00 | 13.28 | H | C |
| ATOM | 1968 | CD1 | ILE | 69 | 103.226 | 19.848 | 15.206 | 1.00 | 13.28 | H | C |
| ATOM | 1969 | C | ILE | 69 | 100.287 | 23.096 | 16.336 | 1.00 | 22.74 | H | C |
| ATOM | 1970 | O | ILE | 69 | 100.282 | 24.065 | 15.578 | 1.00 | 22.74 | H | O |
| ATOM | 1971 | N | SER | 70 | 100.632 | 23.188 | 17.608 | 1.00 | 15.22 | H | N |

Fig. 19: A-28

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1972 | CA | SER | 70 | 101.032 | 24.460 | 18.183 | 1.00 | 15.22 | H | C |
| ATOM | 1973 | CB | SER | 70 | 99.834 | 25.147 | 18.851 | 1.00 | 3.12 | H | C |
| ATOM | 1974 | OG | SER | 70 | 99.588 | 24.606 | 20.144 | 1.00 | 3.12 | H | O |
| ATOM | 1975 | C | SER | 70 | 102.088 | 24.203 | 19.235 | 1.00 | 15.22 | H | C |
| ATOM | 1976 | O | SER | 70 | 102.392 | 23.053 | 19.557 | 1.00 | 15.22 | H | O |
| ATOM | 1977 | N | ARG | 71 | 102.636 | 25.281 | 19.780 | 1.00 | 42.13 | H | N |
| ATOM | 1978 | CA | ARG | 71 | 103.640 | 25.158 | 20.813 | 1.00 | 42.13 | H | C |
| ATOM | 1979 | CB | ARG | 71 | 105.039 | 25.089 | 20.210 | 1.00 | 12.52 | H | C |
| ATOM | 1980 | CG | ARG | 71 | 105.417 | 26.296 | 19.388 | 1.00 | 12.52 | H | C |
| ATOM | 1981 | CD | ARG | 71 | 106.906 | 26.507 | 19.436 | 1.00 | 12.52 | H | C |
| ATOM | 1982 | NE | ARG | 71 | 107.644 | 25.627 | 18.540 | 1.00 | 12.52 | H | N |
| ATOM | 1983 | CZ | ARG | 71 | 108.844 | 25.114 | 18.816 | 1.00 | 12.52 | H | C |
| ATOM | 1984 | NH1 | ARG | 71 | 109.444 | 25.380 | 19.970 | 1.00 | 12.52 | H | N |
| ATOM | 1985 | NH2 | ARG | 71 | 109.456 | 24.354 | 17.924 | 1.00 | 12.52 | H | N |
| ATOM | 1986 | C | ARG | 71 | 103.568 | 26.341 | 21.739 | 1.00 | 42.13 | H | C |
| ATOM | 1987 | O | ARG | 71 | 103.115 | 27.416 | 21.352 | 1.00 | 42.13 | H | O |
| ATOM | 1988 | N | ASP | 72 | 104.003 | 26.131 | 22.973 | 1.00 | 26.38 | H | N |
| ATOM | 1989 | CA | ASP | 72 | 104.034 | 27.197 | 23.954 | 1.00 | 26.38 | H | C |
| ATOM | 1990 | CB | ASP | 72 | 102.949 | 27.026 | 25.007 | 1.00 | 47.03 | H | C |
| ATOM | 1991 | CG | ASP | 72 | 103.003 | 28.108 | 26.050 | 1.00 | 47.03 | H | C |
| ATOM | 1992 | OD1 | ASP | 72 | 102.157 | 28.112 | 26.964 | 1.00 | 47.03 | H | O |
| ATOM | 1993 | OD2 | ASP | 72 | 103.907 | 28.959 | 25.953 | 1.00 | 47.03 | H | O |
| ATOM | 1994 | C | ASP | 72 | 105.402 | 27.159 | 24.607 | 1.00 | 26.38 | H | C |
| ATOM | 1995 | O | ASP | 72 | 105.618 | 26.508 | 25.633 | 1.00 | 26.38 | H | O |
| ATOM | 1996 | N | ASN | 73 | 106.325 | 27.868 | 23.979 | 1.00 | 50.64 | H | N |
| ATOM | 1997 | CA | ASN | 73 | 107.692 | 27.939 | 24.441 | 1.00 | 50.64 | H | C |
| ATOM | 1998 | CB | ASN | 73 | 108.522 | 28.747 | 23.446 | 1.00 | 30.24 | H | C |
| ATOM | 1999 | CG | ASN | 73 | 108.584 | 28.091 | 22.086 | 1.00 | 30.24 | H | C |
| ATOM | 2000 | OD1 | ASN | 73 | 109.170 | 28.625 | 21.149 | 1.00 | 30.24 | H | O |
| ATOM | 2001 | ND2 | ASN | 73 | 107.984 | 26.917 | 21.974 | 1.00 | 30.24 | H | N |
| ATOM | 2002 | C | ASN | 73 | 107.827 | 28.516 | 25.841 | 1.00 | 50.64 | H | C |
| ATOM | 2003 | O | ASN | 73 | 108.898 | 28.436 | 26.438 | 1.00 | 50.64 | H | O |
| ATOM | 2004 | N | SER | 74 | 106.758 | 29.097 | 26.376 | 1.00 | 33.75 | H | N |
| ATOM | 2005 | CA | SER | 74 | 106.848 | 29.644 | 27.723 | 1.00 | 33.75 | H | C |
| ATOM | 2006 | CB | SER | 74 | 105.593 | 30.429 | 28.093 | 1.00 | 48.57 | H | C |
| ATOM | 2007 | OG | SER | 74 | 104.534 | 29.556 | 28.444 | 1.00 | 48.57 | H | O |
| ATOM | 2008 | C | SER | 74 | 106.979 | 28.456 | 28.653 | 1.00 | 33.75 | H | C |
| ATOM | 2009 | O | SER | 74 | 107.681 | 28.530 | 29.660 | 1.00 | 33.75 | H | O |
| ATOM | 2010 | N | LYS | 75 | 106.312 | 27.354 | 28.302 | 1.00 | 39.57 | H | N |
| ATOM | 2011 | CA | LYS | 75 | 106.352 | 26.142 | 29.119 | 1.00 | 39.57 | H | C |
| ATOM | 2012 | CB | LYS | 75 | 104.973 | 25.889 | 29.732 | 1.00 | 42.48 | H | C |
| ATOM | 2013 | CG | LYS | 75 | 103.842 | 25.924 | 28.731 | 1.00 | 42.48 | H | C |
| ATOM | 2014 | CD | LYS | 75 | 102.482 | 25.985 | 29.418 | 1.00 | 42.48 | H | C |
| ATOM | 2015 | CE | LYS | 75 | 102.156 | 27.393 | 29.918 | 1.00 | 42.48 | H | C |
| ATOM | 2016 | NZ | LYS | 75 | 103.090 | 27.928 | 30.963 | 1.00 | 42.48 | H | N |
| ATOM | 2017 | C | LYS | 75 | 106.843 | 24.894 | 28.380 | 1.00 | 39.57 | H | C |
| ATOM | 2018 | O | LYS | 75 | 106.497 | 23.767 | 28.744 | 1.00 | 39.57 | H | O |
| ATOM | 2019 | N | ASN | 76 | 107.660 | 25.110 | 27.353 | 1.00 | 44.84 | H | N |
| ATOM | 2020 | CA | ASN | 76 | 108.245 | 24.043 | 26.539 | 1.00 | 44.84 | H | C |
| ATOM | 2021 | CB | ASN | 76 | 109.572 | 23.608 | 27.139 | 1.00 | 31.30 | H | C |
| ATOM | 2022 | CG | ASN | 76 | 110.528 | 24.766 | 27.312 | 1.00 | 31.30 | H | C |
| ATOM | 2023 | OD1 | ASN | 76 | 111.666 | 24.593 | 27.739 | 1.00 | 31.30 | H | O |
| ATOM | 2024 | ND2 | ASN | 76 | 110.067 | 25.965 | 26.979 | 1.00 | 31.30 | H | N |
| ATOM | 2025 | C | ASN | 76 | 107.362 | 22.827 | 26.322 | 1.00 | 44.84 | H | C |
| ATOM | 2026 | O | ASN | 76 | 107.793 | 21.681 | 26.479 | 1.00 | 44.84 | H | O |
| ATOM | 2027 | N | THR | 77 | 106.121 | 23.090 | 25.941 | 1.00 | 30.42 | H | N |
| ATOM | 2028 | CA | THR | 77 | 105.181 | 22.032 | 25.686 | 1.00 | 30.42 | H | C |
| ATOM | 2029 | CB | THR | 77 | 103.989 | 22.131 | 26.628 | 1.00 | 46.49 | H | C |
| ATOM | 2030 | OG1 | THR | 77 | 104.446 | 21.977 | 27.974 | 1.00 | 46.49 | H | O |
| ATOM | 2031 | CG2 | THR | 77 | 102.975 | 21.045 | 26.319 | 1.00 | 46.49 | H | C |
| ATOM | 2032 | C | THR | 77 | 104.708 | 22.182 | 24.254 | 1.00 | 30.42 | H | C |
| ATOM | 2033 | O | THR | 77 | 104.488 | 23.291 | 23.786 | 1.00 | 30.42 | H | O |
| ATOM | 2034 | N | LEU | 78 | 104.583 | 21.056 | 23.563 | 1.00 | 20.66 | H | N |
| ATOM | 2035 | CA | LEU | 78 | 104.135 | 21.017 | 22.185 | 1.00 | 20.66 | H | C |
| ATOM | 2036 | CB | LEU | 78 | 104.978 | 20.024 | 21.394 | 1.00 | 19.59 | H | C |
| ATOM | 2037 | CG | LEU | 78 | 104.550 | 19.758 | 19.953 | 1.00 | 19.59 | H | C |
| ATOM | 2038 | CD1 | LEU | 78 | 104.575 | 21.055 | 19.166 | 1.00 | 19.59 | H | C |
| ATOM | 2039 | CD2 | LEU | 78 | 105.470 | 18.731 | 19.320 | 1.00 | 19.59 | H | C |
| ATOM | 2040 | C | LEU | 78 | 102.716 | 20.520 | 22.298 | 1.00 | 20.66 | H | C |
| ATOM | 2041 | O | LEU | 78 | 102.368 | 19.921 | 23.312 | 1.00 | 20.66 | H | O |
| ATOM | 2042 | N | TYR | 79 | 101.902 | 20.753 | 21.271 | 1.00 | 30.75 | H | N |
| ATOM | 2043 | CA | TYR | 79 | 100.498 | 20.333 | 21.294 | 1.00 | 30.75 | H | C |
| ATOM | 2044 | CB | TYR | 79 | 99.591 | 21.494 | 21.728 | 1.00 | 47.95 | H | C |

Fig. 19: A-29

| | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2045 | CG | TYR | 79 | 99.809 | 22.008 | 23.119 | 1.00 | 47.95 | H | C |
| ATOM | 2046 | CD1 | TYR | 79 | 99.166 | 21.430 | 24.205 | 1.00 | 47.95 | H | C |
| ATOM | 2047 | CE1 | TYR | 79 | 99.357 | 21.916 | 25.491 | 1.00 | 47.95 | H | C |
| ATOM | 2048 | CD2 | TYR | 79 | 100.655 | 23.085 | 23.349 | 1.00 | 47.95 | H | C |
| ATOM | 2049 | CE2 | TYR | 79 | 100.857 | 23.579 | 24.628 | 1.00 | 47.95 | H | C |
| ATOM | 2050 | CZ | TYR | 79 | 100.204 | 22.991 | 25.695 | 1.00 | 47.95 | H | C |
| ATOM | 2051 | OH | TYR | 79 | 100.404 | 23.493 | 26.958 | 1.00 | 47.95 | H | O |
| ATOM | 2052 | C | TYR | 79 | 99.966 | 19.863 | 19.950 | 1.00 | 30.75 | H | C |
| ATOM | 2053 | O | TYR | 79 | 100.418 | 20.316 | 18.898 | 1.00 | 30.75 | H | O |
| ATOM | 2054 | N | LEU | 80 | 98.981 | 18.969 | 20.003 | 1.00 | 19.83 | H | N |
| ATOM | 2055 | CA | LEU | 80 | 98.308 | 18.472 | 18.811 | 1.00 | 19.83 | H | C |
| ATOM | 2056 | CB | LEU | 80 | 98.776 | 17.070 | 18.397 | 1.00 | 5.08 | H | C |
| ATOM | 2057 | CG | LEU | 80 | 98.132 | 16.598 | 17.076 | 1.00 | 5.08 | H | C |
| ATOM | 2058 | CD1 | LEU | 80 | 98.706 | 17.386 | 15.914 | 1.00 | 5.08 | H | C |
| ATOM | 2059 | CD2 | LEU | 80 | 98.352 | 15.111 | 16.874 | 1.00 | 5.08 | H | C |
| ATOM | 2060 | C | LEU | 80 | 96.838 | 18.411 | 19.182 | 1.00 | 19.83 | H | C |
| ATOM | 2061 | O | LEU | 80 | 96.398 | 17.503 | 19.879 | 1.00 | 19.83 | H | O |
| ATOM | 2062 | N | GLN | 81 | 96.091 | 19.412 | 18.742 | 1.00 | 24.43 | H | N |
| ATOM | 2063 | CA | GLN | 81 | 94.671 | 19.463 | 19.004 | 1.00 | 24.43 | H | C |
| ATOM | 2064 | CB | GLN | 81 | 94.169 | 20.911 | 18.966 | 1.00 | 60.73 | H | C |
| ATOM | 2065 | CG | GLN | 81 | 92.710 | 21.093 | 19.399 | 1.00 | 60.73 | H | C |
| ATOM | 2066 | CD | GLN | 81 | 92.505 | 20.974 | 20.911 | 1.00 | 60.73 | H | C |
| ATOM | 2067 | OE1 | GLN | 81 | 92.981 | 21.810 | 21.691 | 1.00 | 60.73 | H | O |
| ATOM | 2068 | NE2 | GLN | 81 | 91.787 | 19.935 | 21.328 | 1.00 | 60.73 | H | N |
| ATOM | 2069 | C | GLN | 81 | 94.064 | 18.672 | 17.867 | 1.00 | 24.43 | H | C |
| ATOM | 2070 | O | GLN | 81 | 94.376 | 18.921 | 16.698 | 1.00 | 24.43 | H | O |
| ATOM | 2071 | N | MET | 82 | 93.205 | 17.718 | 18.210 | 1.00 | 35.69 | H | N |
| ATOM | 2072 | CA | MET | 82 | 92.559 | 16.878 | 17.211 | 1.00 | 35.69 | H | C |
| ATOM | 2073 | CB | MET | 82 | 92.989 | 15.424 | 17.383 | 1.00 | 24.95 | H | C |
| ATOM | 2074 | CG | MET | 82 | 94.481 | 15.209 | 17.363 | 1.00 | 24.95 | H | C |
| ATOM | 2075 | SD | MET | 82 | 94.896 | 13.491 | 17.609 | 1.00 | 24.95 | H | S |
| ATOM | 2076 | CE | MET | 82 | 94.985 | 13.427 | 19.373 | 1.00 | 24.95 | H | C |
| ATOM | 2077 | C | MET | 82 | 91.051 | 16.957 | 17.316 | 1.00 | 35.69 | H | C |
| ATOM | 2078 | O | MET | 82 | 90.479 | 16.599 | 18.338 | 1.00 | 35.69 | H | O |
| ATOM | 2079 | N | ASN | 83 | 90.414 | 17.416 | 16.247 | 1.00 | 28.29 | H | N |
| ATOM | 2080 | CA | ASN | 83 | 88.968 | 17.536 | 16.204 | 1.00 | 28.29 | H | C |
| ATOM | 2081 | CB | ASN | 83 | 88.550 | 18.989 | 15.985 | 1.00 | 66.28 | H | C |
| ATOM | 2082 | CG | ASN | 83 | 89.274 | 19.943 | 16.899 | 1.00 | 66.28 | H | C |
| ATOM | 2083 | OD1 | ASN | 83 | 89.213 | 19.819 | 18.121 | 1.00 | 66.28 | H | O |
| ATOM | 2084 | ND2 | ASN | 83 | 89.970 | 20.910 | 16.309 | 1.00 | 66.28 | H | N |
| ATOM | 2085 | C | ASN | 83 | 88.502 | 16.728 | 15.025 | 1.00 | 28.29 | H | C |
| ATOM | 2086 | O | ASN | 83 | 89.306 | 16.348 | 14.185 | 1.00 | 28.29 | H | O |
| ATOM | 2087 | N | SER | 84 | 87.199 | 16.486 | 14.954 | 1.00 | 57.41 | H | N |
| ATOM | 2088 | CA | SER | 84 | 86.618 | 15.739 | 13.847 | 1.00 | 57.41 | H | C |
| ATOM | 2089 | CB | SER | 84 | 86.648 | 16.584 | 12.574 | 1.00 | 29.12 | H | C |
| ATOM | 2090 | OG | SER | 84 | 86.027 | 17.836 | 12.786 | 1.00 | 29.12 | H | O |
| ATOM | 2091 | C | SER | 84 | 87.374 | 14.450 | 13.603 | 1.00 | 57.41 | H | C |
| ATOM | 2092 | O | SER | 84 | 87.642 | 14.085 | 12.456 | 1.00 | 57.41 | H | O |
| ATOM | 2093 | N | LEU | 85 | 87.725 | 13.769 | 14.687 | 1.00 | 32.34 | H | N |
| ATOM | 2094 | CA | LEU | 85 | 88.452 | 12.513 | 14.595 | 1.00 | 32.34 | H | C |
| ATOM | 2095 | CB | LEU | 85 | 88.818 | 12.009 | 15.990 | 1.00 | 15.22 | H | C |
| ATOM | 2096 | CG | LEU | 85 | 89.913 | 12.880 | 16.600 | 1.00 | 15.22 | H | C |
| ATOM | 2097 | CD1 | LEU | 85 | 90.082 | 12.594 | 18.078 | 1.00 | 15.22 | H | C |
| ATOM | 2098 | CD2 | LEU | 85 | 91.204 | 12.636 | 15.828 | 1.00 | 15.22 | H | C |
| ATOM | 2099 | C | LEU | 85 | 87.641 | 11.460 | 13.877 | 1.00 | 32.34 | H | C |
| ATOM | 2100 | O | LEU | 85 | 86.434 | 11.369 | 14.050 | 1.00 | 32.34 | H | O |
| ATOM | 2101 | N | ARG | 86 | 88.319 | 10.680 | 13.049 | 1.00 | 24.27 | H | N |
| ATOM | 2102 | CA | ARG | 86 | 87.686 | 9.604 | 12.316 | 1.00 | 24.27 | H | C |
| ATOM | 2103 | CB | ARG | 86 | 87.858 | 9.801 | 10.815 | 1.00 | 51.87 | H | C |
| ATOM | 2104 | CG | ARG | 86 | 87.146 | 11.026 | 10.286 | 1.00 | 51.87 | H | C |
| ATOM | 2105 | CD | ARG | 86 | 86.864 | 10.887 | 8.808 | 1.00 | 51.87 | H | C |
| ATOM | 2106 | NE | ARG | 86 | 87.237 | 12.088 | 8.076 | 1.00 | 51.87 | H | N |
| ATOM | 2107 | CZ | ARG | 86 | 88.470 | 12.581 | 8.043 | 1.00 | 51.87 | H | C |
| ATOM | 2108 | NH1 | ARG | 86 | 89.444 | 11.967 | 8.707 | 1.00 | 51.87 | H | N |
| ATOM | 2109 | NH2 | ARG | 86 | 88.733 | 13.676 | 7.334 | 1.00 | 51.87 | H | N |
| ATOM | 2110 | C | ARG | 86 | 88.387 | 8.343 | 12.769 | 1.00 | 24.27 | H | C |
| ATOM | 2111 | O | ARG | 86 | 89.367 | 8.416 | 13.514 | 1.00 | 24.27 | H | O |
| ATOM | 2112 | N | ALA | 87 | 87.894 | 7.191 | 12.335 | 1.00 | 40.98 | H | N |
| ATOM | 2113 | CA | ALA | 87 | 88.499 | 5.928 | 12.733 | 1.00 | 40.98 | H | C |
| ATOM | 2114 | CB | ALA | 87 | 87.678 | 4.763 | 12.196 | 1.00 | 28.01 | H | C |
| ATOM | 2115 | C | ALA | 87 | 89.937 | 5.833 | 12.242 | 1.00 | 40.98 | H | C |
| ATOM | 2116 | O | ALA | 87 | 90.824 | 5.425 | 12.989 | 1.00 | 40.98 | H | O |
| ATOM | 2117 | N | GLU | 88 | 90.169 | 6.222 | 10.993 | 1.00 | 32.24 | H | N |

Fig. 19: A-30

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2118 | CA | GLU | 88 | 91.511 | 6.157 | 10.433 | 1.00 | 32.24 | H | C |
| ATOM | 2119 | CB | GLU | 88 | 91.583 | 6.890 | 9.094 | 1.00 | 72.38 | H | C |
| ATOM | 2120 | CG | GLU | 88 | 90.432 | 6.614 | 8.169 | 1.00 | 72.38 | H | C |
| ATOM | 2121 | CD | GLU | 88 | 89.327 | 7.623 | 8.336 | 1.00 | 72.38 | H | C |
| ATOM | 2122 | OE1 | GLU | 88 | 89.529 | 8.792 | 7.937 | 1.00 | 72.38 | H | O |
| ATOM | 2123 | OE2 | GLU | 88 | 88.265 | 7.246 | 8.874 | 1.00 | 72.38 | H | O |
| ATOM | 2124 | C | GLU | 88 | 92.529 | 6.780 | 11.372 | 1.00 | 32.24 | H | C |
| ATOM | 2125 | O | GLU | 88 | 93.691 | 6.370 | 11.417 | 1.00 | 32.24 | H | O |
| ATOM | 2126 | N | ASP | 89 | 92.080 | 7.772 | 12.128 | 1.00 | 18.63 | H | N |
| ATOM | 2127 | CA | ASP | 89 | 92.935 | 8.497 | 13.054 | 1.00 | 18.63 | H | C |
| ATOM | 2128 | CB | ASP | 89 | 92.212 | 9.764 | 13.507 | 1.00 | 29.25 | H | C |
| ATOM | 2129 | CG | ASP | 89 | 92.073 | 10.775 | 12.392 | 1.00 | 29.25 | H | C |
| ATOM | 2130 | OD1 | ASP | 89 | 91.297 | 11.732 | 12.553 | 1.00 | 29.25 | H | O |
| ATOM | 2131 | OD2 | ASP | 89 | 92.748 | 10.622 | 11.355 | 1.00 | 29.25 | H | O |
| ATOM | 2132 | C | ASP | 89 | 93.434 | 7.724 | 14.268 | 1.00 | 18.63 | H | C |
| ATOM | 2133 | O | ASP | 89 | 94.391 | 8.149 | 14.922 | 1.00 | 18.63 | H | O |
| ATOM | 2134 | N | THR | 90 | 92.817 | 6.588 | 14.575 | 1.00 | 29.66 | H | N |
| ATOM | 2135 | CA | THR | 90 | 93.261 | 5.845 | 15.749 | 1.00 | 29.66 | H | C |
| ATOM | 2136 | CB | THR | 90 | 92.303 | 4.668 | 16.113 | 1.00 | 30.61 | H | C |
| ATOM | 2137 | OG1 | THR | 90 | 92.601 | 3.537 | 15.293 | 1.00 | 30.61 | H | O |
| ATOM | 2138 | CG2 | THR | 90 | 90.828 | 5.072 | 15.903 | 1.00 | 30.61 | H | C |
| ATOM | 2139 | C | THR | 90 | 94.664 | 5.311 | 15.527 | 1.00 | 29.66 | H | C |
| ATOM | 2140 | O | THR | 90 | 94.961 | 4.727 | 14.492 | 1.00 | 29.66 | H | O |
| ATOM | 2141 | N | ALA | 91 | 95.532 | 5.553 | 16.499 | 1.00 | 11.25 | H | N |
| ATOM | 2142 | CA | ALA | 91 | 96.918 | 5.094 | 16.451 | 1.00 | 11.25 | H | C |
| ATOM | 2143 | CB | ALA | 91 | 97.629 | 5.690 | 15.259 | 1.00 | 1.87 | H | C |
| ATOM | 2144 | C | ALA | 91 | 97.611 | 5.536 | 17.729 | 1.00 | 11.25 | H | C |
| ATOM | 2145 | O | ALA | 91 | 96.972 | 6.044 | 18.646 | 1.00 | 11.25 | H | O |
| ATOM | 2146 | N | VAL | 92 | 98.915 | 5.312 | 17.797 | 1.00 | 22.44 | H | N |
| ATOM | 2147 | CA | VAL | 92 | 99.694 | 5.755 | 18.947 | 1.00 | 22.44 | H | C |
| ATOM | 2148 | CB | VAL | 92 | 100.654 | 4.665 | 19.465 | 1.00 | 21.44 | H | C |
| ATOM | 2149 | CG1 | VAL | 92 | 101.306 | 3.966 | 18.298 | 1.00 | 21.44 | H | C |
| ATOM | 2150 | CG2 | VAL | 92 | 101.716 | 5.284 | 20.346 | 1.00 | 21.44 | H | C |
| ATOM | 2151 | C | VAL | 92 | 100.482 | 6.913 | 18.363 | 1.00 | 22.44 | H | C |
| ATOM | 2152 | O | VAL | 92 | 101.107 | 6.771 | 17.310 | 1.00 | 22.44 | H | O |
| ATOM | 2153 | N | TYR | 93 | 100.413 | 8.066 | 19.019 | 1.00 | 21.58 | H | N |
| ATOM | 2154 | CA | TYR | 93 | 101.105 | 9.261 | 18.538 | 1.00 | 21.58 | H | C |
| ATOM | 2155 | CB | TYR | 93 | 100.161 | 10.470 | 18.585 | 1.00 | 12.38 | H | C |
| ATOM | 2156 | CG | TYR | 93 | 99.000 | 10.385 | 17.624 | 1.00 | 12.38 | H | C |
| ATOM | 2157 | CD1 | TYR | 93 | 98.023 | 9.399 | 17.759 | 1.00 | 12.38 | H | C |
| ATOM | 2158 | CE1 | TYR | 93 | 96.975 | 9.287 | 16.836 | 1.00 | 12.38 | H | C |
| ATOM | 2159 | CD2 | TYR | 93 | 98.899 | 11.264 | 16.553 | 1.00 | 12.38 | H | C |
| ATOM | 2160 | CE2 | TYR | 93 | 97.863 | 11.165 | 15.634 | 1.00 | 12.38 | H | C |
| ATOM | 2161 | CZ | TYR | 93 | 96.908 | 10.173 | 15.773 | 1.00 | 12.38 | H | C |
| ATOM | 2162 | OH | TYR | 93 | 95.915 | 10.043 | 14.827 | 1.00 | 12.38 | H | O |
| ATOM | 2163 | C | TYR | 93 | 102.384 | 9.577 | 19.312 | 1.00 | 21.58 | H | C |
| ATOM | 2164 | O | TYR | 93 | 102.466 | 9.401 | 20.531 | 1.00 | 21.58 | H | O |
| ATOM | 2165 | N | TYR | 94 | 103.381 | 10.049 | 18.579 | 1.00 | 19.04 | H | N |
| ATOM | 2166 | CA | TYR | 94 | 104.668 | 10.409 | 19.151 | 1.00 | 19.04 | H | C |
| ATOM | 2167 | CB | TYR | 94 | 105.789 | 9.576 | 18.533 | 1.00 | 29.80 | H | C |
| ATOM | 2168 | CG | TYR | 94 | 105.548 | 8.101 | 18.431 | 1.00 | 29.80 | H | C |
| ATOM | 2169 | CD1 | TYR | 94 | 105.948 | 7.237 | 19.454 | 1.00 | 29.80 | H | C |
| ATOM | 2170 | CE1 | TYR | 94 | 105.768 | 5.876 | 19.345 | 1.00 | 29.80 | H | C |
| ATOM | 2171 | CD2 | TYR | 94 | 104.958 | 7.563 | 17.298 | 1.00 | 29.80 | H | C |
| ATOM | 2172 | CE2 | TYR | 94 | 104.773 | 6.204 | 17.177 | 1.00 | 29.80 | H | C |
| ATOM | 2173 | CZ | TYR | 94 | 105.179 | 5.363 | 18.202 | 1.00 | 29.80 | H | C |
| ATOM | 2174 | OH | TYR | 94 | 104.996 | 4.007 | 18.071 | 1.00 | 29.80 | H | O |
| ATOM | 2175 | C | TYR | 94 | 104.991 | 11.853 | 18.805 | 1.00 | 19.04 | H | C |
| ATOM | 2176 | O | TYR | 94 | 104.867 | 12.244 | 17.642 | 1.00 | 19.04 | H | O |
| ATOM | 2177 | N | CYS | 95 | 105.383 | 12.654 | 19.791 | 1.00 | 25.07 | H | N |
| ATOM | 2178 | CA | CYS | 95 | 105.806 | 14.000 | 19.466 | 1.00 | 25.07 | H | C |
| ATOM | 2179 | C | CYS | 95 | 107.228 | 13.689 | 19.096 | 1.00 | 25.07 | H | C |
| ATOM | 2180 | O | CYS | 95 | 107.716 | 12.584 | 19.342 | 1.00 | 25.07 | H | O |
| ATOM | 2181 | CB | CYS | 95 | 105.784 | 14.942 | 20.647 | 1.00 | 46.53 | H | C |
| ATOM | 2182 | SG | CYS | 95 | 106.112 | 14.206 | 22.267 | 1.00 | 46.53 | H | S |
| ATOM | 2183 | N | THR | 96 | 107.931 | 14.657 | 18.549 | 1.00 | 31.61 | H | N |
| ATOM | 2184 | CA | THR | 96 | 109.253 | 14.331 | 18.115 | 1.00 | 31.61 | H | C |
| ATOM | 2185 | CB | THR | 96 | 109.088 | 13.445 | 16.861 | 1.00 | 32.15 | H | C |
| ATOM | 2186 | OG1 | THR | 96 | 110.331 | 12.862 | 16.494 | 1.00 | 32.15 | H | O |
| ATOM | 2187 | CG2 | THR | 96 | 108.554 | 14.260 | 15.708 | 1.00 | 32.15 | H | C |
| ATOM | 2188 | C | THR | 96 | 110.045 | 15.591 | 17.830 | 1.00 | 31.61 | H | C |
| ATOM | 2189 | O | THR | 96 | 109.530 | 16.548 | 17.260 | 1.00 | 31.61 | H | O |
| ATOM | 2190 | N | ARG | 97 | 111.292 | 15.610 | 18.270 | 1.00 | 26.02 | H | N |

Fig. 19: A-31

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2191 | CA | ARG | 97 | 112.135 | 16.759 | 17.996 | 1.00 | 26.02 | H | C |
| ATOM | 2192 | CB | ARG | 97 | 113.220 | 16.959 | 19.053 | 1.00 | 22.53 | H | C |
| ATOM | 2193 | CG | ARG | 97 | 114.076 | 18.184 | 18.766 | 1.00 | 22.53 | H | C |
| ATOM | 2194 | CD | ARG | 97 | 115.204 | 18.345 | 19.764 | 1.00 | 22.53 | H | C |
| ATOM | 2195 | NE | ARG | 97 | 116.357 | 17.532 | 19.411 | 1.00 | 22.53 | H | N |
| ATOM | 2196 | CZ | ARG | 97 | 117.494 | 17.509 | 20.099 | 1.00 | 22.53 | H | C |
| ATOM | 2197 | NH1 | ARG | 97 | 117.635 | 18.257 | 21.183 | 1.00 | 22.53 | H | N |
| ATOM | 2198 | NH2 | ARG | 97 | 118.494 | 16.739 | 19.704 | 1.00 | 22.53 | H | N |
| ATOM | 2199 | C | ARG | 97 | 112.799 | 16.473 | 16.665 | 1.00 | 26.02 | H | C |
| ATOM | 2200 | O | ARG | 97 | 113.145 | 15.322 | 16.357 | 1.00 | 26.02 | H | O |
| ATOM | 2201 | N | GLY | 98 | 112.980 | 17.528 | 15.882 | 1.00 | 13.43 | H | N |
| ATOM | 2202 | CA | GLY | 98 | 113.586 | 17.367 | 14.582 | 1.00 | 13.43 | H | C |
| ATOM | 2203 | C | GLY | 98 | 114.947 | 17.995 | 14.496 | 1.00 | 13.43 | H | C |
| ATOM | 2204 | O | GLY | 98 | 115.308 | 18.850 | 15.281 | 1.00 | 13.43 | H | O |
| ATOM | 2205 | N | PHE | 99 | 115.719 | 17.537 | 13.534 | 1.00 | 20.13 | H | N |
| ATOM | 2206 | CA | PHE | 99 | 117.038 | 18.065 | 13.315 | 1.00 | 20.13 | H | C |
| ATOM | 2207 | CB | PHE | 99 | 118.018 | 16.902 | 13.211 | 1.00 | 25.23 | H | C |
| ATOM | 2208 | CG | PHE | 99 | 119.338 | 17.271 | 12.628 | 1.00 | 25.23 | H | C |
| ATOM | 2209 | CD1 | PHE | 99 | 119.587 | 17.079 | 11.279 | 1.00 | 25.23 | H | C |
| ATOM | 2210 | CD2 | PHE | 99 | 120.326 | 17.828 | 13.420 | 1.00 | 25.23 | H | C |
| ATOM | 2211 | CE1 | PHE | 99 | 120.804 | 17.437 | 10.721 | 1.00 | 25.23 | H | C |
| ATOM | 2212 | CE2 | PHE | 99 | 121.543 | 18.191 | 12.875 | 1.00 | 25.23 | H | C |
| ATOM | 2213 | CZ | PHE | 99 | 121.784 | 17.994 | 11.517 | 1.00 | 25.23 | H | C |
| ATOM | 2214 | C | PHE | 99 | 116.887 | 18.819 | 11.996 | 1.00 | 20.13 | H | C |
| ATOM | 2215 | O | PHE | 99 | 115.950 | 18.551 | 11.241 | 1.00 | 20.13 | H | O |
| ATOM | 2216 | N | GLY | 100 | 117.768 | 19.774 | 11.719 | 1.00 | 15.08 | H | N |
| ATOM | 2217 | CA | GLY | 100 | 117.655 | 20.513 | 10.469 | 1.00 | 15.08 | H | C |
| ATOM | 2218 | C | GLY | 100 | 116.285 | 21.139 | 10.274 | 1.00 | 15.08 | H | C |
| ATOM | 2219 | O | GLY | 100 | 115.682 | 21.636 | 11.216 | 1.00 | 15.08 | H | O |
| ATOM | 2220 | N | ASP | 101 | 115.779 | 21.128 | 9.050 | 1.00 | 7.89 | H | N |
| ATOM | 2221 | CA | ASP | 101 | 114.462 | 21.692 | 8.812 | 1.00 | 7.89 | H | C |
| ATOM | 2222 | CB | ASP | 101 | 114.195 | 21.848 | 7.302 | 1.00 | 13.13 | H | C |
| ATOM | 2223 | CG | ASP | 101 | 115.328 | 22.587 | 6.564 | 1.00 | 13.13 | H | C |
| ATOM | 2224 | OD1 | ASP | 101 | 115.921 | 23.558 | 7.105 | 1.00 | 13.13 | H | O |
| ATOM | 2225 | OD2 | ASP | 101 | 115.616 | 22.190 | 5.417 | 1.00 | 13.13 | H | O |
| ATOM | 2226 | C | ASP | 101 | 113.406 | 20.785 | 9.460 | 1.00 | 7.89 | H | C |
| ATOM | 2227 | O | ASP | 101 | 112.222 | 20.844 | 9.124 | 1.00 | 7.89 | H | O |
| ATOM | 2228 | N | GLY | 102 | 113.854 | 19.924 | 10.374 | 1.00 | 22.31 | H | N |
| ATOM | 2229 | CA | GLY | 102 | 112.952 | 19.043 | 11.100 | 1.00 | 22.31 | H | C |
| ATOM | 2230 | C | GLY | 102 | 112.588 | 17.674 | 10.562 | 1.00 | 22.31 | H | C |
| ATOM | 2231 | O | GLY | 102 | 111.927 | 16.915 | 11.263 | 1.00 | 22.31 | H | O |
| ATOM | 2232 | N | GLY | 103 | 113.001 | 17.347 | 9.343 | 1.00 | 25.09 | H | N |
| ATOM | 2233 | CA | GLY | 103 | 112.662 | 16.054 | 8.772 | 1.00 | 25.09 | H | C |
| ATOM | 2234 | C | GLY | 103 | 113.342 | 14.844 | 9.403 | 1.00 | 25.09 | H | C |
| ATOM | 2235 | O | GLY | 103 | 112.948 | 13.703 | 9.156 | 1.00 | 25.09 | H | O |
| ATOM | 2236 | N | TYR | 104 | 114.376 | 15.071 | 10.202 | 1.00 | 22.52 | H | N |
| ATOM | 2237 | CA | TYR | 104 | 115.070 | 13.961 | 10.844 | 1.00 | 22.52 | H | C |
| ATOM | 2238 | CB | TYR | 104 | 116.578 | 14.114 | 10.715 | 1.00 | 15.87 | H | C |
| ATOM | 2239 | CG | TYR | 104 | 117.342 | 13.175 | 11.599 | 1.00 | 15.87 | H | C |
| ATOM | 2240 | CD1 | TYR | 104 | 118.507 | 13.600 | 12.233 | 1.00 | 15.87 | H | C |
| ATOM | 2241 | CE1 | TYR | 104 | 119.198 | 12.776 | 13.100 | 1.00 | 15.87 | H | C |
| ATOM | 2242 | CD2 | TYR | 104 | 116.884 | 11.880 | 11.844 | 1.00 | 15.87 | H | C |
| ATOM | 2243 | CE2 | TYR | 104 | 117.575 | 11.034 | 12.713 | 1.00 | 15.87 | H | C |
| ATOM | 2244 | CZ | TYR | 104 | 118.734 | 11.498 | 13.343 | 1.00 | 15.87 | H | C |
| ATOM | 2245 | OH | TYR | 104 | 119.417 | 10.713 | 14.239 | 1.00 | 15.87 | H | O |
| ATOM | 2246 | C | TYR | 104 | 114.665 | 13.991 | 12.296 | 1.00 | 22.52 | H | C |
| ATOM | 2247 | O | TYR | 104 | 114.933 | 14.956 | 13.001 | 1.00 | 22.52 | H | O |
| ATOM | 2248 | N | PHE | 105 | 114.036 | 12.909 | 12.733 | 1.00 | 16.00 | H | N |
| ATOM | 2249 | CA | PHE | 105 | 113.501 | 12.806 | 14.073 | 1.00 | 16.00 | H | C |
| ATOM | 2250 | CB | PHE | 105 | 112.292 | 11.890 | 14.031 | 1.00 | 16.01 | H | C |
| ATOM | 2251 | CG | PHE | 105 | 111.269 | 12.327 | 13.020 | 1.00 | 16.01 | H | C |
| ATOM | 2252 | CD1 | PHE | 105 | 110.782 | 13.627 | 13.038 | 1.00 | 16.01 | H | C |
| ATOM | 2253 | CD2 | PHE | 105 | 110.827 | 11.459 | 12.023 | 1.00 | 16.01 | H | C |
| ATOM | 2254 | CE1 | PHE | 105 | 109.880 | 14.059 | 12.091 | 1.00 | 16.01 | H | C |
| ATOM | 2255 | CE2 | PHE | 105 | 109.918 | 11.885 | 11.067 | 1.00 | 16.01 | H | C |
| ATOM | 2256 | CZ | PHE | 105 | 109.443 | 13.190 | 11.101 | 1.00 | 16.01 | H | C |
| ATOM | 2257 | C | PHE | 105 | 114.442 | 12.433 | 15.179 | 1.00 | 16.00 | H | C |
| ATOM | 2258 | O | PHE | 105 | 114.543 | 11.283 | 15.595 | 1.00 | 16.00 | H | O |
| ATOM | 2259 | N | ASP | 106 | 115.105 | 13.481 | 15.642 | 1.00 | 29.40 | H | N |
| ATOM | 2260 | CA | ASP | 106 | 116.089 | 13.519 | 16.714 | 1.00 | 29.40 | H | C |
| ATOM | 2261 | CB | ASP | 106 | 116.251 | 14.976 | 17.117 | 1.00 | 39.43 | H | C |
| ATOM | 2262 | CG | ASP | 106 | 117.656 | 15.400 | 17.133 | 1.00 | 39.43 | H | C |
| ATOM | 2263 | OD1 | ASP | 106 | 118.492 | 14.528 | 17.433 | 1.00 | 39.43 | H | O |

Fig. 19: A-32

```
ATOM   2264  OD2 ASP   106     117.922  16.591  16.859  1.00  39.43      H     O
ATOM   2265  C   ASP   106     115.797  12.728  17.993  1.00  29.40      H     C
ATOM   2266  O   ASP   106     116.567  11.861  18.396  1.00  29.40      H     O
ATOM   2267  N   VAL   107     114.687  13.094  18.635  1.00   7.69      H     N
ATOM   2268  CA  VAL   107     114.248  12.533  19.906  1.00   7.69      H     C
ATOM   2269  CB  VAL   107     114.402  13.600  21.026  1.00  10.61      H     C
ATOM   2270  CG1 VAL   107     113.985  13.045  22.374  1.00  10.61      H     C
ATOM   2271  CG2 VAL   107     115.838  14.116  21.048  1.00  10.61      H     C
ATOM   2272  C   VAL   107     112.778  12.199  19.765  1.00   7.69      H     C
ATOM   2273  O   VAL   107     112.107  12.835  18.970  1.00   7.69      H     O
ATOM   2274  N   TRP   108     112.285  11.224  20.540  1.00  26.84      H     N
ATOM   2275  CA  TRP   108     110.871  10.795  20.510  1.00  26.84      H     C
ATOM   2276  CB  TRP   108     110.729   9.405  19.868  1.00   1.87      H     C
ATOM   2277  CG  TRP   108     111.201   9.329  18.468  1.00   1.87      H     C
ATOM   2278  CD2 TRP   108     110.431   8.950  17.328  1.00   1.87      H     C
ATOM   2279  CE2 TRP   108     111.287   9.020  16.201  1.00   1.87      H     C
ATOM   2280  CE3 TRP   108     109.102   8.557  17.142  1.00   1.87      H     C
ATOM   2281  CD1 TRP   108     112.460   9.606  18.008  1.00   1.87      H     C
ATOM   2282  NE1 TRP   108     112.520   9.422  16.648  1.00   1.87      H     N
ATOM   2283  CZ2 TRP   108     110.854   8.710  14.904  1.00   1.87      H     C
ATOM   2284  CZ3 TRP   108     108.667   8.244  15.836  1.00   1.87      H     C
ATOM   2285  CH2 TRP   108     109.547   8.325  14.742  1.00   1.87      H     C
ATOM   2286  C   TRP   108     110.204  10.724  21.881  1.00  26.84      H     C
ATOM   2287  O   TRP   108     110.859  10.503  22.899  1.00  26.84      H     O
ATOM   2288  N   GLY   109     108.889  10.907  21.889  1.00  15.55      H     N
ATOM   2289  CA  GLY   109     108.134  10.811  23.125  1.00  15.55      H     C
ATOM   2290  C   GLY   109     107.896   9.331  23.386  1.00  15.55      H     C
ATOM   2291  O   GLY   109     108.170   8.502  22.511  1.00  15.55      H     O
ATOM   2292  N   GLN   110     107.393   8.971  24.563  1.00  21.92      H     N
ATOM   2293  CA  GLN   110     107.161   7.554  24.852  1.00  21.92      H     C
ATOM   2294  CB  GLN   110     106.800   7.338  26.325  1.00  44.26      H     C
ATOM   2295  CG  GLN   110     105.404   7.798  26.703  1.00  44.26      H     C
ATOM   2296  CD  GLN   110     105.321   9.283  26.957  1.00  44.26      H     C
ATOM   2297  OE1 GLN   110     105.573  10.102  26.071  1.00  44.26      H     O
ATOM   2298  NE2 GLN   110     104.967   9.642  28.181  1.00  44.26      H     N
ATOM   2299  C   GLN   110     106.051   6.979  23.973  1.00  21.92      H     C
ATOM   2300  O   GLN   110     106.054   5.798  23.651  1.00  21.92      H     O
ATOM   2301  N   GLY   111     105.114   7.824  23.574  1.00  22.63      H     N
ATOM   2302  CA  GLY   111     104.014   7.361  22.761  1.00  22.63      H     C
ATOM   2303  C   GLY   111     102.758   7.463  23.597  1.00  22.63      H     C
ATOM   2304  O   GLY   111     102.834   7.414  24.827  1.00  22.63      H     O
ATOM   2305  N   THR   112     101.611   7.619  22.938  1.00  17.52      H     N
ATOM   2306  CA  THR   112     100.333   7.740  23.630  1.00  17.52      H     C
ATOM   2307  CB  THR   112     100.058   9.211  24.030  1.00  34.98      H     C
ATOM   2308  OG1 THR   112      98.958   9.261  24.939  1.00  34.98      H     O
ATOM   2309  CG2 THR   112      99.734  10.055  22.809  1.00  34.98      H     C
ATOM   2310  C   THR   112      99.228   7.203  22.717  1.00  17.52      H     C
ATOM   2311  O   THR   112      99.133   7.559  21.533  1.00  17.52      H     O
ATOM   2312  N   LEU   113      98.396   6.340  23.292  1.00  32.82      H     N
ATOM   2313  CA  LEU   113      97.318   5.668  22.576  1.00  32.82      H     C
ATOM   2314  CB  LEU   113      96.953   4.374  23.328  1.00  26.98      H     C
ATOM   2315  CG  LEU   113      95.842   3.431  22.856  1.00  26.98      H     C
ATOM   2316  CD1 LEU   113      94.455   4.057  23.105  1.00  26.98      H     C
ATOM   2317  CD2 LEU   113      96.055   3.115  21.392  1.00  26.98      H     C
ATOM   2318  C   LEU   113      96.073   6.498  22.354  1.00  32.82      H     C
ATOM   2319  O   LEU   113      95.448   6.964  23.299  1.00  32.82      H     O
ATOM   2320  N   VAL   114      95.708   6.671  21.094  1.00  38.48      H     N
ATOM   2321  CA  VAL   114      94.506   7.419  20.767  1.00  38.48      H     C
ATOM   2322  CB  VAL   114      94.809   8.658  19.870  1.00  53.69      H     C
ATOM   2323  CG1 VAL   114      93.518   9.420  19.571  1.00  53.69      H     C
ATOM   2324  CG2 VAL   114      95.798   9.575  20.562  1.00  53.69      H     C
ATOM   2325  C   VAL   114      93.557   6.484  20.022  1.00  38.48      H     C
ATOM   2326  O   VAL   114      93.859   6.003  18.928  1.00  38.48      H     O
ATOM   2327  N   THR   115      92.411   6.216  20.629  1.00  29.76      H     N
ATOM   2328  CA  THR   115      91.414   5.356  20.012  1.00  29.76      H     C
ATOM   2329  CB  THR   115      91.081   4.125  20.916  1.00  30.84      H     C
ATOM   2330  OG1 THR   115      92.292   3.453  21.300  1.00  30.84      H     O
ATOM   2331  CG2 THR   115      90.180   3.151  20.170  1.00  30.84      H     C
ATOM   2332  C   THR   115      90.133   6.164  19.803  1.00  29.76      H     C
ATOM   2333  O   THR   115      89.700   6.905  20.694  1.00  29.76      H     O
ATOM   2334  N   VAL   116      89.543   6.056  18.619  1.00  38.29      H     N
ATOM   2335  CA  VAL   116      88.289   6.747  18.371  1.00  38.29      H     C
ATOM   2336  CB  VAL   116      88.395   7.822  17.240  1.00  10.28      H     C
```

Fig. 19: A-33

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2337 | CG1 | VAL | 116 | 89.861 | 8.088 | 16.922 | 1.00 | 10.28 | H | C |
| ATOM | 2338 | CG2 | VAL | 116 | 87.575 | 7.415 | 15.994 | 1.00 | 10.28 | H | C |
| ATOM | 2339 | C | VAL | 116 | 87.303 | 5.656 | 17.996 | 1.00 | 38.29 | H | C |
| ATOM | 2340 | O | VAL | 116 | 87.545 | 4.888 | 17.063 | 1.00 | 38.29 | H | O |
| ATOM | 2341 | N | SER | 117 | 86.207 | 5.579 | 18.746 | 1.00 | 41.53 | H | N |
| ATOM | 2342 | CA | SER | 117 | 85.193 | 4.565 | 18.517 | 1.00 | 41.53 | H | C |
| ATOM | 2343 | CB | SER | 117 | 85.768 | 3.182 | 18.851 | 1.00 | 61.62 | H | C |
| ATOM | 2344 | OG | SER | 117 | 84.788 | 2.165 | 18.751 | 1.00 | 61.62 | H | O |
| ATOM | 2345 | C | SER | 117 | 83.959 | 4.815 | 19.366 | 1.00 | 41.53 | H | C |
| ATOM | 2346 | O | SER | 117 | 84.049 | 5.336 | 20.482 | 1.00 | 41.53 | H | O |
| ATOM | 2347 | N | SER | 118 | 82.808 | 4.431 | 18.828 | 1.00 | 36.79 | H | N |
| ATOM | 2348 | CA | SER | 118 | 81.538 | 4.581 | 19.525 | 1.00 | 36.79 | H | C |
| ATOM | 2349 | CB | SER | 118 | 80.401 | 4.226 | 18.579 | 1.00 | 49.30 | H | C |
| ATOM | 2350 | OG | SER | 118 | 80.598 | 2.919 | 18.069 | 1.00 | 49.30 | H | O |
| ATOM | 2351 | C | SER | 118 | 81.510 | 3.649 | 20.740 | 1.00 | 36.79 | H | C |
| ATOM | 2352 | O | SER | 118 | 80.753 | 3.853 | 21.685 | 1.00 | 35.84 | H | O |
| ATOM | 2353 | N | ALA | 119 | 82.339 | 2.616 | 20.707 | 1.00 | 26.31 | H | N |
| ATOM | 2354 | CA | ALA | 119 | 82.412 | 1.679 | 21.815 | 1.00 | 26.31 | H | C |
| ATOM | 2355 | CB | ALA | 119 | 83.569 | 0.707 | 21.617 | 1.00 | 20.55 | H | C |
| ATOM | 2356 | C | ALA | 119 | 82.611 | 2.461 | 23.100 | 1.00 | 26.31 | H | C |
| ATOM | 2357 | O | ALA | 119 | 83.319 | 3.477 | 23.124 | 1.00 | 26.31 | H | O |
| ATOM | 2358 | N | SER | 120 | 81.988 | 1.975 | 24.166 | 1.00 | 39.08 | H | N |
| ATOM | 2359 | CA | SER | 120 | 82.074 | 2.621 | 25.462 | 1.00 | 39.08 | H | C |
| ATOM | 2360 | CB | SER | 120 | 80.711 | 2.597 | 26.151 | 1.00 | 57.76 | H | C |
| ATOM | 2361 | OG | SER | 120 | 79.720 | 3.179 | 25.329 | 1.00 | 57.76 | H | O |
| ATOM | 2362 | C | SER | 120 | 83.086 | 1.938 | 26.353 | 1.00 | 39.08 | H | C |
| ATOM | 2363 | O | SER | 120 | 83.194 | 0.715 | 26.362 | 1.00 | 39.08 | H | O |
| ATOM | 2364 | N | THR | 121 | 83.837 | 2.734 | 27.100 | 1.00 | 26.62 | H | N |
| ATOM | 2365 | CA | THR | 121 | 84.813 | 2.188 | 28.023 | 1.00 | 25.63 | H | C |
| ATOM | 2366 | CB | THR | 121 | 85.274 | 3.267 | 29.002 | 1.00 | 27.79 | H | C |
| ATOM | 2367 | OG1 | THR | 121 | 85.860 | 4.353 | 28.268 | 1.00 | 32.58 | H | O |
| ATOM | 2368 | CG2 | THR | 121 | 86.273 | 2.691 | 30.007 | 1.00 | 25.52 | H | C |
| ATOM | 2369 | C | THR | 121 | 84.108 | 1.078 | 28.801 | 1.00 | 26.35 | H | C |
| ATOM | 2370 | O | THR | 121 | 82.919 | 1.189 | 29.098 | 1.00 | 29.95 | H | O |
| ATOM | 2371 | N | LYS | 122 | 84.828 | 0.007 | 29.116 | 1.00 | 53.26 | H | N |
| ATOM | 2372 | CA | LYS | 122 | 84.243 | -1.102 | 29.864 | 1.00 | 50.64 | H | C |
| ATOM | 2373 | CB | LYS | 122 | 83.333 | -1.930 | 28.947 | 1.00 | 42.70 | H | C |
| ATOM | 2374 | CG | LYS | 122 | 83.009 | -3.347 | 29.437 | 1.00 | 44.07 | H | C |
| ATOM | 2375 | CD | LYS | 122 | 82.469 | -3.373 | 30.864 | 1.00 | 47.16 | H | C |
| ATOM | 2376 | CE | LYS | 122 | 82.216 | -4.805 | 31.337 | 1.00 | 51.36 | H | C |
| ATOM | 2377 | NZ | LYS | 122 | 81.986 | -4.880 | 32.809 | 1.00 | 50.23 | H | N |
| ATOM | 2378 | C | LYS | 122 | 85.301 | -1.991 | 30.496 | 1.00 | 52.40 | H | C |
| ATOM | 2379 | O | LYS | 122 | 86.154 | -2.548 | 29.809 | 1.00 | 54.02 | H | O |
| ATOM | 2380 | N | GLY | 123 | 85.240 | -2.114 | 31.817 | 1.00 | 42.56 | H | N |
| ATOM | 2381 | CA | GLY | 123 | 86.188 | -2.952 | 32.530 | 1.00 | 42.89 | H | C |
| ATOM | 2382 | C | GLY | 123 | 86.213 | -4.396 | 32.035 | 1.00 | 44.35 | H | C |
| ATOM | 2383 | O | GLY | 123 | 85.222 | -4.907 | 31.503 | 1.00 | 40.33 | H | O |
| ATOM | 2384 | N | PRO | 124 | 87.346 | -5.090 | 32.198 | 1.00 | 44.81 | H | N |
| ATOM | 2385 | CD | PRO | 124 | 88.680 | -4.632 | 32.633 | 1.00 | 21.78 | H | C |
| ATOM | 2386 | CA | PRO | 124 | 87.397 | -6.472 | 31.731 | 1.00 | 46.19 | H | C |
| ATOM | 2387 | CB | PRO | 124 | 88.868 | -6.668 | 31.439 | 1.00 | 22.93 | H | C |
| ATOM | 2388 | CG | PRO | 124 | 89.504 | -5.905 | 32.561 | 1.00 | 22.69 | H | C |
| ATOM | 2389 | C | PRO | 124 | 86.899 | -7.461 | 32.764 | 1.00 | 45.69 | H | C |
| ATOM | 2390 | O | PRO | 124 | 86.854 | -7.170 | 33.961 | 1.00 | 46.94 | H | O |
| ATOM | 2391 | N | SER | 125 | 86.507 | -8.631 | 32.287 | 1.00 | 43.49 | H | N |
| ATOM | 2392 | CA | SER | 125 | 86.053 | -9.678 | 33.176 | 1.00 | 38.23 | H | C |
| ATOM | 2393 | CB | SER | 125 | 84.858 | -10.416 | 32.579 | 1.00 | 23.34 | H | C |
| ATOM | 2394 | OG | SER | 125 | 83.756 | -9.544 | 32.402 | 1.00 | 25.34 | H | O |
| ATOM | 2395 | C | SER | 125 | 87.262 | -10.576 | 33.200 | 1.00 | 33.52 | H | C |
| ATOM | 2396 | O | SER | 125 | 87.738 | -10.972 | 32.139 | 1.00 | 32.91 | H | O |
| ATOM | 2397 | N | VAL | 126 | 87.787 | -10.873 | 34.386 | 1.00 | 23.96 | H | N |
| ATOM | 2398 | CA | VAL | 126 | 88.962 | -11.727 | 34.452 | 1.00 | 20.86 | H | C |
| ATOM | 2399 | CB | VAL | 126 | 90.135 | -11.003 | 35.174 | 1.00 | 22.19 | H | C |
| ATOM | 2400 | CG1 | VAL | 126 | 89.894 | -9.504 | 35.113 | 1.00 | 17.46 | H | C |
| ATOM | 2401 | CG2 | VAL | 126 | 90.331 | -11.507 | 36.597 | 1.00 | 22.90 | H | C |
| ATOM | 2402 | C | VAL | 126 | 88.666 | -13.091 | 35.065 | 1.00 | 20.51 | H | C |
| ATOM | 2403 | O | VAL | 126 | 88.382 | -13.227 | 36.256 | 1.00 | 24.79 | H | O |
| ATOM | 2404 | N | PHE | 127 | 88.713 | -14.105 | 34.213 | 1.00 | 27.15 | H | N |
| ATOM | 2405 | CA | PHE | 127 | 88.443 | -15.464 | 34.625 | 1.00 | 29.56 | H | C |
| ATOM | 2406 | CB | PHE | 127 | 87.628 | -16.167 | 33.544 | 1.00 | 16.06 | H | C |
| ATOM | 2407 | CG | PHE | 127 | 86.392 | -15.419 | 33.141 | 1.00 | 12.41 | H | C |
| ATOM | 2408 | CD1 | PHE | 127 | 85.380 | -15.167 | 34.071 | 1.00 | 11.21 | H | C |
| ATOM | 2409 | CD2 | PHE | 127 | 86.255 | -14.922 | 31.840 | 1.00 | 10.06 | H | C |

Fig. 19: A-34

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2410 | CE1 | PHE | 127 | 84.254 | -14.428 | 33.721 | 1.00 | 12.93 | H | C |
| ATOM | 2411 | CE2 | PHE | 127 | 85.126 | -14.174 | 31.470 | 1.00 | 6.89 | H | C |
| ATOM | 2412 | CZ | PHE | 127 | 84.125 | -13.925 | 32.413 | 1.00 | 6.94 | H | C |
| ATOM | 2413 | C | PHE | 127 | 89.763 | -16.183 | 34.825 | 1.00 | 31.37 | H | C |
| ATOM | 2414 | O | PHE | 127 | 90.806 | -15.733 | 34.351 | 1.00 | 34.05 | H | O |
| ATOM | 2415 | N | PRO | 128 | 89.743 | -17.310 | 35.540 | 1.00 | 21.35 | H | N |
| ATOM | 2416 | CD | PRO | 128 | 88.681 | -17.812 | 36.434 | 1.00 | 32.37 | H | C |
| ATOM | 2417 | CA | PRO | 128 | 90.996 | -18.039 | 35.752 | 1.00 | 22.25 | H | C |
| ATOM | 2418 | CB | PRO | 128 | 90.823 | -18.577 | 37.161 | 1.00 | 34.03 | H | C |
| ATOM | 2419 | CG | PRO | 128 | 89.358 | -18.983 | 37.130 | 1.00 | 33.18 | H | C |
| ATOM | 2420 | C | PRO | 128 | 91.198 | -19.176 | 34.739 | 1.00 | 21.65 | H | C |
| ATOM | 2421 | O | PRO | 128 | 90.235 | -19.770 | 34.244 | 1.00 | 21.29 | H | O |
| ATOM | 2422 | N | LEU | 129 | 92.457 | -19.457 | 34.432 | 1.00 | 17.17 | H | N |
| ATOM | 2423 | CA | LEU | 129 | 92.811 | -20.557 | 33.545 | 1.00 | 19.61 | H | C |
| ATOM | 2424 | CB | LEU | 129 | 93.683 | -20.061 | 32.396 | 1.00 | 18.81 | H | C |
| ATOM | 2425 | CG | LEU | 129 | 93.086 | -18.872 | 31.635 | 1.00 | 18.17 | H | C |
| ATOM | 2426 | CD1 | LEU | 129 | 94.115 | -18.254 | 30.696 | 1.00 | 16.12 | H | C |
| ATOM | 2427 | CD2 | LEU | 129 | 91.886 | -19.341 | 30.870 | 1.00 | 11.94 | H | C |
| ATOM | 2428 | C | LEU | 129 | 93.601 | -21.457 | 34.497 | 1.00 | 23.45 | H | C |
| ATOM | 2429 | O | LEU | 129 | 94.824 | -21.481 | 34.499 | 1.00 | 25.82 | H | O |
| ATOM | 2430 | N | ALA | 130 | 92.870 | -22.179 | 35.332 | 1.00 | 16.93 | H | N |
| ATOM | 2431 | CA | ALA | 130 | 93.455 | -23.046 | 36.341 | 1.00 | 18.97 | H | C |
| ATOM | 2432 | CB | ALA | 130 | 92.363 | -23.561 | 37.256 | 1.00 | 49.82 | H | C |
| ATOM | 2433 | C | ALA | 130 | 94.280 | -24.219 | 35.846 | 1.00 | 18.88 | H | C |
| ATOM | 2434 | O | ALA | 130 | 93.928 | -24.876 | 34.869 | 1.00 | 20.61 | H | O |
| ATOM | 2435 | N | PRO | 131 | 95.401 | -24.490 | 36.534 | 1.00 | 29.98 | H | N |
| ATOM | 2436 | CD | PRO | 131 | 95.929 | -23.703 | 37.665 | 1.00 | 16.68 | H | C |
| ATOM | 2437 | CA | PRO | 131 | 96.301 | -25.595 | 36.198 | 1.00 | 27.20 | H | C |
| ATOM | 2438 | CB | PRO | 131 | 97.453 | -25.424 | 37.196 | 1.00 | 12.88 | H | C |
| ATOM | 2439 | CG | PRO | 131 | 96.815 | -24.691 | 38.354 | 1.00 | 15.86 | H | C |
| ATOM | 2440 | C | PRO | 131 | 95.534 | -26.897 | 36.405 | 1.00 | 26.68 | H | C |
| ATOM | 2441 | O | PRO | 131 | 94.666 | -26.978 | 37.274 | 1.00 | 27.16 | H | O |
| ATOM | 2442 | N | SER | 132 | 95.838 | -27.912 | 35.607 | 1.00 | 64.88 | H | N |
| ATOM | 2443 | CA | SER | 132 | 95.138 | -29.187 | 35.720 | 1.00 | 67.56 | H | C |
| ATOM | 2444 | CB | SER | 132 | 93.745 | -29.075 | 35.086 | 1.00 | 44.77 | H | C |
| ATOM | 2445 | OG | SER | 132 | 93.824 | -28.747 | 33.704 | 1.00 | 46.53 | H | O |
| ATOM | 2446 | C | SER | 132 | 95.918 | -30.284 | 35.020 | 1.00 | 69.15 | H | C |
| ATOM | 2447 | O | SER | 132 | 97.107 | -30.139 | 34.757 | 1.00 | 69.80 | H | O |
| ATOM | 2448 | N | SER | 133 | 95.247 | -31.391 | 34.732 | 1.00 | 58.75 | H | N |
| ATOM | 2449 | CA | SER | 133 | 95.894 | -32.483 | 34.024 | 1.00 | 61.13 | H | C |
| ATOM | 2450 | CB | SER | 133 | 95.007 | -33.738 | 34.068 | 1.00 | 91.14 | H | C |
| ATOM | 2451 | OG | SER | 133 | 93.668 | -33.456 | 33.684 | 1.00 | 100.88 | H | O |
| ATOM | 2452 | C | SER | 133 | 96.121 | -32.017 | 32.576 | 1.00 | 60.76 | H | C |
| ATOM | 2453 | O | SER | 133 | 97.091 | -32.413 | 31.927 | 1.00 | 61.01 | H | O |
| ATOM | 2454 | N | LYS | 134 | 95.220 | -31.156 | 32.095 | 1.00 | 101.65 | H | N |
| ATOM | 2455 | CA | LYS | 134 | 95.285 | -30.605 | 30.739 | 1.00 | 102.79 | H | C |
| ATOM | 2456 | CB | LYS | 134 | 93.951 | -29.962 | 30.341 | 1.00 | 44.82 | H | C |
| ATOM | 2457 | CG | LYS | 134 | 92.703 | -30.784 | 30.609 | 1.00 | 52.94 | H | C |
| ATOM | 2458 | CD | LYS | 134 | 92.058 | -30.452 | 31.959 | 1.00 | 55.86 | H | C |
| ATOM | 2459 | CE | LYS | 134 | 90.686 | -31.127 | 32.091 | 1.00 | 53.71 | H | C |
| ATOM | 2460 | NZ | LYS | 134 | 89.988 | -30.792 | 33.367 | 1.00 | 52.28 | H | N |
| ATOM | 2461 | C | LYS | 134 | 96.364 | -29.531 | 30.655 | 1.00 | 102.96 | H | C |
| ATOM | 2462 | O | LYS | 134 | 96.932 | -29.284 | 29.589 | 1.00 | 104.03 | H | O |
| ATOM | 2463 | N | SER | 135 | 96.619 | -28.885 | 31.791 | 1.00 | 77.03 | H | N |
| ATOM | 2464 | CA | SER | 135 | 97.611 | -27.818 | 31.896 | 1.00 | 76.76 | H | C |
| ATOM | 2465 | CB | SER | 135 | 97.069 | -26.698 | 32.784 | 1.00 | 81.66 | H | C |
| ATOM | 2466 | OG | SER | 135 | 95.726 | -26.390 | 32.443 | 1.00 | 81.07 | H | O |
| ATOM | 2467 | C | SER | 135 | 98.911 | -28.358 | 32.488 | 1.00 | 71.98 | H | C |
| ATOM | 2468 | O | SER | 135 | 99.733 | -27.601 | 33.006 | 1.00 | 72.29 | H | O |
| ATOM | 2469 | N | THR | 136 | 99.075 | -29.676 | 32.418 | 1.00 | 86.02 | H | N |
| ATOM | 2470 | CA | THR | 136 | 100.262 | -30.351 | 32.932 | 1.00 | 86.44 | H | C |
| ATOM | 2471 | CB | THR | 136 | 99.897 | -31.391 | 34.036 | 1.00 | 47.16 | H | C |
| ATOM | 2472 | OG1 | THR | 136 | 99.491 | -30.715 | 35.237 | 1.00 | 47.25 | H | O |
| ATOM | 2473 | CG2 | THR | 136 | 101.096 | -32.281 | 34.354 | 1.00 | 50.70 | H | C |
| ATOM | 2474 | C | THR | 136 | 100.977 | -31.072 | 31.788 | 1.00 | 86.90 | H | C |
| ATOM | 2475 | O | THR | 136 | 100.334 | -31.615 | 30.885 | 1.00 | 85.81 | H | O |
| ATOM | 2476 | N | SER | 137 | 102.309 | -31.059 | 31.836 | 1.00 | 82.54 | H | N |
| ATOM | 2477 | CA | SER | 137 | 103.164 | -31.700 | 30.834 | 1.00 | 82.34 | H | C |
| ATOM | 2478 | CB | SER | 137 | 103.113 | -30.942 | 29.495 | 1.00 | 65.40 | H | C |
| ATOM | 2479 | OG | SER | 137 | 101.863 | -31.097 | 28.841 | 1.00 | 66.87 | H | O |
| ATOM | 2480 | C | SER | 137 | 104.600 | -31.715 | 31.352 | 1.00 | 82.68 | H | C |
| ATOM | 2481 | O | SER | 137 | 105.321 | -30.722 | 31.244 | 1.00 | 84.11 | H | O |
| ATOM | 2482 | N | GLY | 138 | 105.016 | -32.845 | 31.911 | 1.00 | 62.73 | H | N |

Fig. 19: A-35

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2483 | CA | GLY | 138 | 106.361 | -32.941 | 32.438 | 1.00 | 62.79 | H | C |
| ATOM | 2484 | C | GLY | 138 | 106.394 | -32.371 | 33.840 | 1.00 | 65.01 | H | C |
| ATOM | 2485 | O | GLY | 138 | 105.392 | -32.410 | 34.555 | 1.00 | 65.52 | H | O |
| ATOM | 2486 | N | GLY | 139 | 107.537 | -31.827 | 34.237 | 1.00 | 45.62 | H | N |
| ATOM | 2487 | CA | GLY | 139 | 107.645 | -31.267 | 35.570 | 1.00 | 45.97 | H | C |
| ATOM | 2488 | C | GLY | 139 | 107.037 | -29.884 | 35.680 | 1.00 | 46.52 | H | C |
| ATOM | 2489 | O | GLY | 139 | 107.020 | -29.297 | 36.762 | 1.00 | 50.66 | H | O |
| ATOM | 2490 | N | THR | 140 | 106.527 | -29.365 | 34.568 | 1.00 | 41.37 | H | N |
| ATOM | 2491 | CA | THR | 140 | 105.941 | -28.030 | 34.571 | 1.00 | 35.80 | H | C |
| ATOM | 2492 | CB | THR | 140 | 106.626 | -27.108 | 33.533 | 1.00 | 32.97 | H | C |
| ATOM | 2493 | OG1 | THR | 140 | 105.886 | -27.138 | 32.311 | 1.00 | 30.01 | H | O |
| ATOM | 2494 | CG2 | THR | 140 | 108.052 | -27.574 | 33.250 | 1.00 | 33.92 | H | C |
| ATOM | 2495 | C | THR | 140 | 104.434 | -27.993 | 34.299 | 1.00 | 32.68 | H | C |
| ATOM | 2496 | O | THR | 140 | 103.884 | -28.820 | 33.560 | 1.00 | 31.27 | H | O |
| ATOM | 2497 | N | ALA | 141 | 103.777 | -27.013 | 34.914 | 1.00 | 23.19 | H | N |
| ATOM | 2498 | CA | ALA | 141 | 102.350 | -26.817 | 34.752 | 1.00 | 23.90 | H | C |
| ATOM | 2499 | CB | ALA | 141 | 101.647 | -26.986 | 36.087 | 1.00 | 31.87 | H | C |
| ATOM | 2500 | C | ALA | 141 | 102.121 | -25.408 | 34.206 | 1.00 | 24.06 | H | C |
| ATOM | 2501 | O | ALA | 141 | 102.930 | -24.498 | 34.415 | 1.00 | 28.34 | H | O |
| ATOM | 2502 | N | ALA | 142 | 101.022 | -25.239 | 33.487 | 1.00 | 36.28 | H | N |
| ATOM | 2503 | CA | ALA | 142 | 100.685 | -23.948 | 32.924 | 1.00 | 31.12 | H | C |
| ATOM | 2504 | CB | ALA | 142 | 100.507 | -24.062 | 31.419 | 1.00 | 1.87 | H | C |
| ATOM | 2505 | C | ALA | 142 | 99.389 | -23.519 | 33.588 | 1.00 | 29.11 | H | C |
| ATOM | 2506 | O | ALA | 142 | 98.565 | -24.359 | 33.961 | 1.00 | 33.50 | H | O |
| ATOM | 2507 | N | LEU | 143 | 99.233 | -22.211 | 33.751 | 1.00 | 27.06 | H | N |
| ATOM | 2508 | CA | LEU | 143 | 98.054 | -21.611 | 34.372 | 1.00 | 31.22 | H | C |
| ATOM | 2509 | CB | LEU | 143 | 98.154 | -21.670 | 35.900 | 1.00 | 28.24 | H | C |
| ATOM | 2510 | CG | LEU | 143 | 99.269 | -20.865 | 36.582 | 1.00 | 30.55 | H | C |
| ATOM | 2511 | CD1 | LEU | 143 | 98.702 | -19.526 | 36.991 | 1.00 | 23.14 | H | C |
| ATOM | 2512 | CD2 | LEU | 143 | 99.817 | -21.596 | 37.809 | 1.00 | 37.29 | H | C |
| ATOM | 2513 | C | LEU | 143 | 98.068 | -20.169 | 33.913 | 1.00 | 34.46 | H | C |
| ATOM | 2514 | O | LEU | 143 | 99.069 | -19.700 | 33.364 | 1.00 | 32.14 | H | O |
| ATOM | 2515 | N | GLY | 144 | 96.970 | -19.458 | 34.128 | 1.00 | 25.78 | H | N |
| ATOM | 2516 | CA | GLY | 144 | 96.922 | -18.074 | 33.694 | 1.00 | 28.57 | H | C |
| ATOM | 2517 | C | GLY | 144 | 95.578 | -17.425 | 33.896 | 1.00 | 31.81 | H | C |
| ATOM | 2518 | O | GLY | 144 | 94.693 | -17.985 | 34.543 | 1.00 | 35.57 | H | O |
| ATOM | 2519 | N | CYS | 145 | 95.420 | -16.235 | 33.335 | 1.00 | 24.76 | H | N |
| ATOM | 2520 | CA | CYS | 145 | 94.177 | -15.501 | 33.471 | 1.00 | 23.67 | H | C |
| ATOM | 2521 | C | CYS | 145 | 93.665 | -15.071 | 32.122 | 1.00 | 21.65 | H | C |
| ATOM | 2522 | O | CYS | 145 | 94.437 | -14.868 | 31.188 | 1.00 | 22.23 | H | O |
| ATOM | 2523 | CB | CYS | 145 | 94.385 | -14.273 | 34.363 | 1.00 | 28.67 | H | C |
| ATOM | 2524 | SG | CYS | 145 | 94.354 | -14.658 | 36.141 | 1.00 | 36.96 | H | S |
| ATOM | 2525 | N | LEU | 146 | 92.351 | -14.940 | 32.024 | 1.00 | 43.52 | H | N |
| ATOM | 2526 | CA | LEU | 146 | 91.712 | -14.512 | 30.792 | 1.00 | 43.76 | H | C |
| ATOM | 2527 | CB | LEU | 146 | 90.715 | -15.580 | 30.314 | 1.00 | 38.89 | H | C |
| ATOM | 2528 | CG | LEU | 146 | 89.754 | -15.245 | 29.164 | 1.00 | 28.77 | H | C |
| ATOM | 2529 | CD1 | LEU | 146 | 90.519 | -14.669 | 27.982 | 1.00 | 25.69 | H | C |
| ATOM | 2530 | CD2 | LEU | 146 | 88.989 | -16.489 | 28.755 | 1.00 | 35.84 | H | C |
| ATOM | 2531 | C | LEU | 146 | 90.997 | -13.188 | 31.055 | 1.00 | 45.61 | H | C |
| ATOM | 2532 | O | LEU | 146 | 89.943 | -13.160 | 31.690 | 1.00 | 45.79 | H | O |
| ATOM | 2533 | N | VAL | 147 | 91.609 | -12.098 | 30.593 | 1.00 | 12.91 | H | N |
| ATOM | 2534 | CA | VAL | 147 | 91.069 | -10.732 | 30.716 | 1.00 | 12.94 | H | C |
| ATOM | 2535 | CB | VAL | 147 | 92.231 | -9.696 | 30.638 | 1.00 | 24.21 | H | C |
| ATOM | 2536 | CG1 | VAL | 147 | 91.703 | -8.291 | 30.722 | 1.00 | 25.32 | H | C |
| ATOM | 2537 | CG2 | VAL | 147 | 93.212 | -9.947 | 31.778 | 1.00 | 13.52 | H | C |
| ATOM | 2538 | C | VAL | 147 | 90.101 | -10.563 | 29.532 | 1.00 | 18.31 | H | C |
| ATOM | 2539 | O | VAL | 147 | 90.532 | -10.460 | 28.381 | 1.00 | 18.59 | H | O |
| ATOM | 2540 | N | LYS | 148 | 88.798 | -10.519 | 29.806 | 1.00 | 25.16 | H | N |
| ATOM | 2541 | CA | LYS | 148 | 87.835 | -10.467 | 28.709 | 1.00 | 29.22 | H | C |
| ATOM | 2542 | CB | LYS | 148 | 87.140 | -11.827 | 28.609 | 1.00 | 15.56 | H | C |
| ATOM | 2543 | CG | LYS | 148 | 86.353 | -12.032 | 27.348 | 1.00 | 22.92 | H | C |
| ATOM | 2544 | CD | LYS | 148 | 85.731 | -13.405 | 27.355 | 1.00 | 22.16 | H | C |
| ATOM | 2545 | CE | LYS | 148 | 84.795 | -13.570 | 26.190 | 1.00 | 24.54 | H | C |
| ATOM | 2546 | NZ | LYS | 148 | 85.514 | -13.308 | 24.928 | 1.00 | 22.92 | H | N |
| ATOM | 2547 | C | LYS | 148 | 86.777 | -9.372 | 28.646 | 1.00 | 32.79 | H | C |
| ATOM | 2548 | O | LYS | 148 | 86.332 | -8.844 | 29.664 | 1.00 | 33.18 | H | O |
| ATOM | 2549 | N | ASP | 149 | 86.387 | -9.069 | 27.409 | 1.00 | 55.13 | H | N |
| ATOM | 2550 | CA | ASP | 149 | 85.381 | -8.070 | 27.078 | 1.00 | 53.92 | H | C |
| ATOM | 2551 | CB | ASP | 149 | 83.993 | -8.595 | 27.429 | 1.00 | 38.49 | H | C |
| ATOM | 2552 | CG | ASP | 149 | 83.635 | -9.853 | 26.661 | 1.00 | 42.52 | H | C |
| ATOM | 2553 | OD1 | ASP | 149 | 83.797 | -9.882 | 25.421 | 1.00 | 46.52 | H | O |
| ATOM | 2554 | OD2 | ASP | 149 | 83.181 | -10.817 | 27.305 | 1.00 | 41.08 | H | O |
| ATOM | 2555 | C | ASP | 149 | 85.585 | -6.690 | 27.698 | 1.00 | 56.06 | H | C |

Fig. 19: A-36

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2556 | O | ASP | 149 | 84.720 | -6.175 | 28.415 | 1.00 | 57.30 | H | O |
| ATOM | 2557 | N | TYR | 150 | 86.734 | -6.091 | 27.399 | 1.00 | 33.00 | H | N |
| ATOM | 2558 | CA | TYR | 150 | 87.072 | -4.770 | 27.897 | 1.00 | 33.34 | H | C |
| ATOM | 2559 | CB | TYR | 150 | 88.306 | -4.844 | 28.797 | 1.00 | 39.19 | H | C |
| ATOM | 2560 | CG | TYR | 150 | 89.622 | -5.155 | 28.097 | 1.00 | 44.75 | H | C |
| ATOM | 2561 | CD1 | TYR | 150 | 90.405 | -4.137 | 27.556 | 1.00 | 44.06 | H | C |
| ATOM | 2562 | CE1 | TYR | 150 | 91.653 | -4.401 | 26.994 | 1.00 | 46.40 | H | C |
| ATOM | 2563 | CD2 | TYR | 150 | 90.121 | -6.457 | 28.046 | 1.00 | 44.23 | H | C |
| ATOM | 2564 | CE2 | TYR | 150 | 91.369 | -6.730 | 27.483 | 1.00 | 43.19 | H | C |
| ATOM | 2565 | CZ | TYR | 150 | 92.130 | -5.694 | 26.963 | 1.00 | 45.07 | H | C |
| ATOM | 2566 | OH | TYR | 150 | 93.376 | -5.942 | 26.431 | 1.00 | 42.66 | H | O |
| ATOM | 2567 | C | TYR | 150 | 87.331 | -3.838 | 26.723 | 1.00 | 34.19 | H | C |
| ATOM | 2568 | O | TYR | 150 | 87.420 | -4.275 | 25.569 | 1.00 | 36.79 | H | O |
| ATOM | 2569 | N | PHE | 151 | 87.450 | -2.549 | 27.034 | 1.00 | 53.36 | H | N |
| ATOM | 2570 | CA | PHE | 151 | 87.686 | -1.522 | 26.034 | 1.00 | 51.06 | H | C |
| ATOM | 2571 | CB | PHE | 151 | 86.520 | -1.506 | 25.038 | 1.00 | 22.52 | H | C |
| ATOM | 2572 | CG | PHE | 151 | 86.663 | -0.500 | 23.923 | 1.00 | 22.34 | H | C |
| ATOM | 2573 | CD1 | PHE | 151 | 86.509 | 0.865 | 24.164 | 1.00 | 21.58 | H | C |
| ATOM | 2574 | CD2 | PHE | 151 | 86.896 | -0.923 | 22.616 | 1.00 | 24.08 | H | C |
| ATOM | 2575 | CE1 | PHE | 151 | 86.576 | 1.789 | 23.117 | 1.00 | 22.62 | H | C |
| ATOM | 2576 | CE2 | PHE | 151 | 86.968 | -0.003 | 21.558 | 1.00 | 25.39 | H | C |
| ATOM | 2577 | CZ | PHE | 151 | 86.805 | 1.351 | 21.809 | 1.00 | 25.56 | H | C |
| ATOM | 2578 | C | PHE | 151 | 87.819 | -0.175 | 26.734 | 1.00 | 48.17 | H | C |
| ATOM | 2579 | O | PHE | 151 | 87.161 | 0.084 | 27.737 | 1.00 | 47.45 | H | O |
| ATOM | 2580 | N | PRO | 152 | 88.712 | 0.685 | 26.232 | 1.00 | 46.09 | H | N |
| ATOM | 2581 | CD | PRO | 152 | 88.959 | 2.055 | 26.730 | 1.00 | 7.14 | H | C |
| ATOM | 2582 | CA | PRO | 152 | 89.554 | 0.388 | 25.065 | 1.00 | 47.66 | H | C |
| ATOM | 2583 | CB | PRO | 152 | 89.773 | 1.765 | 24.464 | 1.00 | 12.39 | H | C |
| ATOM | 2584 | CG | PRO | 152 | 90.017 | 2.594 | 25.730 | 1.00 | 9.55 | H | C |
| ATOM | 2585 | C | PRO | 152 | 90.835 | -0.199 | 25.636 | 1.00 | 47.42 | H | C |
| ATOM | 2586 | O | PRO | 152 | 90.826 | -0.716 | 26.748 | 1.00 | 49.63 | H | O |
| ATOM | 2587 | N | GLU | 153 | 91.933 | -0.128 | 24.894 | 1.00 | 48.37 | H | N |
| ATOM | 2588 | CA | GLU | 153 | 93.200 | -0.620 | 25.422 | 1.00 | 45.01 | H | C |
| ATOM | 2589 | CB | GLU | 153 | 94.232 | -0.788 | 24.308 | 1.00 | 35.76 | H | C |
| ATOM | 2590 | CG | GLU | 153 | 93.983 | -1.951 | 23.370 | 1.00 | 41.71 | H | C |
| ATOM | 2591 | CD | GLU | 153 | 94.465 | -3.279 | 23.920 | 1.00 | 49.73 | H | C |
| ATOM | 2592 | OE1 | GLU | 153 | 94.329 | -4.276 | 23.191 | 1.00 | 53.96 | H | O |
| ATOM | 2593 | OE2 | GLU | 153 | 94.979 | -3.337 | 25.062 | 1.00 | 49.06 | H | O |
| ATOM | 2594 | C | GLU | 153 | 93.667 | 0.487 | 26.355 | 1.00 | 40.62 | H | C |
| ATOM | 2595 | O | GLU | 153 | 93.160 | 1.611 | 26.288 | 1.00 | 43.09 | H | O |
| ATOM | 2596 | N | PRO | 154 | 94.626 | 0.193 | 27.242 | 1.00 | 31.67 | H | N |
| ATOM | 2597 | CD | PRO | 154 | 95.605 | 1.250 | 27.562 | 1.00 | 24.24 | H | C |
| ATOM | 2598 | CA | PRO | 154 | 95.266 | -1.107 | 27.404 | 1.00 | 32.01 | H | C |
| ATOM | 2599 | CB | PRO | 154 | 96.707 | -0.803 | 27.072 | 1.00 | 23.56 | H | C |
| ATOM | 2600 | CG | PRO | 154 | 96.899 | 0.447 | 27.855 | 1.00 | 23.31 | H | C |
| ATOM | 2601 | C | PRO | 154 | 95.127 | -1.577 | 28.846 | 1.00 | 37.33 | H | C |
| ATOM | 2602 | O | PRO | 154 | 94.929 | -0.788 | 29.770 | 1.00 | 40.93 | H | O |
| ATOM | 2603 | N | VAL | 155 | 95.270 | -2.874 | 29.029 | 1.00 | 27.89 | H | N |
| ATOM | 2604 | CA | VAL | 155 | 95.171 | -3.468 | 30.339 | 1.00 | 28.93 | H | C |
| ATOM | 2605 | CB | VAL | 155 | 94.167 | -4.647 | 30.309 | 1.00 | 32.63 | H | C |
| ATOM | 2606 | CG1 | VAL | 155 | 94.624 | -5.699 | 29.306 | 1.00 | 39.44 | H | C |
| ATOM | 2607 | CG2 | VAL | 155 | 94.030 | -5.243 | 31.690 | 1.00 | 38.09 | H | C |
| ATOM | 2608 | C | VAL | 155 | 96.561 | -3.969 | 30.715 | 1.00 | 29.75 | H | C |
| ATOM | 2609 | O | VAL | 155 | 97.319 | -4.427 | 29.856 | 1.00 | 34.58 | H | O |
| ATOM | 2610 | N | THR | 156 | 96.898 | -3.864 | 31.995 | 1.00 | 30.47 | H | N |
| ATOM | 2611 | CA | THR | 156 | 98.195 | -4.322 | 32.482 | 1.00 | 30.67 | H | C |
| ATOM | 2612 | CB | THR | 156 | 98.855 | -3.316 | 33.458 | 1.00 | 37.06 | H | C |
| ATOM | 2613 | OG1 | THR | 156 | 98.554 | -3.699 | 34.810 | 1.00 | 41.96 | H | O |
| ATOM | 2614 | CG2 | THR | 156 | 98.346 | -1.895 | 33.213 | 1.00 | 35.30 | H | C |
| ATOM | 2615 | C | THR | 156 | 97.956 | -5.589 | 33.276 | 1.00 | 28.26 | H | C |
| ATOM | 2616 | O | THR | 156 | 96.915 | -5.736 | 33.906 | 1.00 | 24.33 | H | O |
| ATOM | 2617 | N | VAL | 157 | 98.914 | -6.501 | 33.250 | 1.00 | 20.40 | H | N |
| ATOM | 2618 | CA | VAL | 157 | 98.784 | -7.731 | 34.014 | 1.00 | 23.86 | H | C |
| ATOM | 2619 | CB | VAL | 157 | 98.263 | -8.918 | 33.149 | 1.00 | 6.55 | H | C |
| ATOM | 2620 | CG1 | VAL | 157 | 98.307 | -10.191 | 33.970 | 1.00 | 2.70 | H | C |
| ATOM | 2621 | CG2 | VAL | 157 | 96.817 | -8.649 | 32.662 | 1.00 | 8.40 | H | C |
| ATOM | 2622 | C | VAL | 157 | 100.122 | -8.142 | 34.618 | 1.00 | 25.91 | H | C |
| ATOM | 2623 | O | VAL | 157 | 101.130 | -8.220 | 33.918 | 1.00 | 28.24 | H | O |
| ATOM | 2624 | N | SER | 158 | 100.127 | -8.401 | 35.918 | 1.00 | 37.92 | H | N |
| ATOM | 2625 | CA | SER | 158 | 101.333 | -8.840 | 36.606 | 1.00 | 38.42 | H | C |
| ATOM | 2626 | CB | SER | 158 | 101.852 | -7.738 | 37.521 | 1.00 | 26.79 | H | C |
| ATOM | 2627 | OG | SER | 158 | 101.008 | -7.591 | 38.648 | 1.00 | 29.78 | H | O |
| ATOM | 2628 | C | SER | 158 | 100.947 | -10.064 | 37.439 | 1.00 | 37.35 | H | C |

Fig. 19: A-37

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2629 | O | SER | 158 | 99.765 | -10.366 | 37.583 | 1.00 | 35.45 | H | O |
| ATOM | 2630 | N | TRP | 159 | 101.926 | -10.772 | 37.989 | 1.00 | 38.23 | H | N |
| ATOM | 2631 | CA | TRP | 159 | 101.604 | -11.945 | 38.790 | 1.00 | 38.96 | H | C |
| ATOM | 2632 | CB | TRP | 159 | 102.060 | -13.224 | 38.074 | 1.00 | 33.06 | H | C |
| ATOM | 2633 | CG | TRP | 159 | 101.197 | -13.555 | 36.899 | 1.00 | 30.80 | H | C |
| ATOM | 2634 | CD2 | TRP | 159 | 100.089 | -14.463 | 36.879 | 1.00 | 31.04 | H | C |
| ATOM | 2635 | CE2 | TRP | 159 | 99.540 | -14.423 | 35.577 | 1.00 | 29.21 | H | C |
| ATOM | 2636 | CE3 | TRP | 159 | 99.507 | -15.307 | 37.836 | 1.00 | 31.84 | H | C |
| ATOM | 2637 | CD1 | TRP | 159 | 101.271 | -13.015 | 35.649 | 1.00 | 26.46 | H | C |
| ATOM | 2638 | NE1 | TRP | 159 | 100.280 | -13.531 | 34.848 | 1.00 | 30.17 | H | N |
| ATOM | 2639 | CZ2 | TRP | 159 | 98.439 | -15.196 | 35.204 | 1.00 | 33.73 | H | C |
| ATOM | 2640 | CZ3 | TRP | 159 | 98.407 | -16.079 | 37.465 | 1.00 | 33.56 | H | C |
| ATOM | 2641 | CH2 | TRP | 159 | 97.887 | -16.018 | 36.158 | 1.00 | 34.95 | H | C |
| ATOM | 2642 | C | TRP | 159 | 102.166 | -11.908 | 40.203 | 1.00 | 41.53 | H | C |
| ATOM | 2643 | O | TRP | 159 | 103.355 | -11.670 | 40.412 | 1.00 | 40.45 | H | O |
| ATOM | 2644 | N | ASN | 160 | 101.295 | -12.163 | 41.170 | 1.00 | 50.63 | H | N |
| ATOM | 2645 | CA | ASN | 160 | 101.699 | -12.153 | 42.557 | 1.00 | 51.18 | H | C |
| ATOM | 2646 | CB | ASN | 160 | 102.753 | -13.230 | 42.814 | 1.00 | 31.23 | H | C |
| ATOM | 2647 | CG | ASN | 160 | 102.145 | -14.619 | 42.946 | 1.00 | 28.65 | H | C |
| ATOM | 2648 | OD1 | ASN | 160 | 100.924 | -14.784 | 42.911 | 1.00 | 22.55 | H | O |
| ATOM | 2649 | ND2 | ASN | 160 | 103.000 | -15.630 | 43.107 | 1.00 | 28.71 | H | N |
| ATOM | 2650 | C | ASN | 160 | 102.245 | -10.777 | 42.891 | 1.00 | 53.56 | H | C |
| ATOM | 2651 | O | ASN | 160 | 103.277 | -10.637 | 43.554 | 1.00 | 51.84 | H | O |
| ATOM | 2652 | N | SER | 161 | 101.548 | -9.758 | 42.397 | 1.00 | 57.36 | H | N |
| ATOM | 2653 | CA | SER | 161 | 101.915 | -8.372 | 42.651 | 1.00 | 58.07 | H | C |
| ATOM | 2654 | CB | SER | 161 | 101.833 | -8.106 | 44.161 | 1.00 | 44.49 | H | C |
| ATOM | 2655 | OG | SER | 161 | 100.611 | -8.586 | 44.713 | 1.00 | 48.26 | H | O |
| ATOM | 2656 | C | SER | 161 | 103.305 | -7.997 | 42.118 | 1.00 | 57.98 | H | C |
| ATOM | 2657 | O | SER | 161 | 103.779 | -6.883 | 42.329 | 1.00 | 58.91 | H | O |
| ATOM | 2658 | N | GLY | 162 | 103.957 | -8.927 | 41.431 | 1.00 | 43.40 | H | N |
| ATOM | 2659 | CA | GLY | 162 | 105.271 | -8.641 | 40.886 | 1.00 | 41.61 | H | C |
| ATOM | 2660 | C | GLY | 162 | 106.343 | -9.670 | 41.195 | 1.00 | 41.13 | H | C |
| ATOM | 2661 | O | GLY | 162 | 107.340 | -9.756 | 40.475 | 1.00 | 41.89 | H | O |
| ATOM | 2662 | N | ALA | 163 | 106.144 | -10.460 | 42.248 | 1.00 | 32.79 | H | N |
| ATOM | 2663 | CA | ALA | 163 | 107.135 | -11.462 | 42.644 | 1.00 | 33.15 | H | C |
| ATOM | 2664 | CB | ALA | 163 | 106.845 | -11.956 | 44.065 | 1.00 | 7.75 | H | C |
| ATOM | 2665 | C | ALA | 163 | 107.265 | -12.651 | 41.702 | 1.00 | 33.69 | H | C |
| ATOM | 2666 | O | ALA | 163 | 108.154 | -13.473 | 41.868 | 1.00 | 36.52 | H | O |
| ATOM | 2667 | N | LEU | 164 | 106.378 | -12.750 | 40.722 | 1.00 | 33.04 | H | N |
| ATOM | 2668 | CA | LEU | 164 | 106.412 | -13.847 | 39.755 | 1.00 | 28.09 | H | C |
| ATOM | 2669 | CB | LEU | 164 | 105.146 | -14.701 | 39.869 | 1.00 | 29.67 | H | C |
| ATOM | 2670 | CG | LEU | 164 | 105.008 | -15.851 | 38.870 | 1.00 | 27.43 | H | C |
| ATOM | 2671 | CD1 | LEU | 164 | 105.976 | -16.963 | 39.215 | 1.00 | 24.01 | H | C |
| ATOM | 2672 | CD2 | LEU | 164 | 103.605 | -16.370 | 38.903 | 1.00 | 22.28 | H | C |
| ATOM | 2673 | C | LEU | 164 | 106.483 | -13.227 | 38.370 | 1.00 | 26.00 | H | C |
| ATOM | 2674 | O | LEU | 164 | 105.492 | -12.663 | 37.893 | 1.00 | 20.06 | H | O |
| ATOM | 2675 | N | THR | 165 | 107.656 | -13.326 | 37.740 | 1.00 | 28.49 | H | N |
| ATOM | 2676 | CA | THR | 165 | 107.893 | -12.758 | 36.410 | 1.00 | 32.54 | H | C |
| ATOM | 2677 | CB | THR | 165 | 108.927 | -11.613 | 36.462 | 1.00 | 18.33 | H | C |
| ATOM | 2678 | OG1 | THR | 165 | 110.114 | -12.057 | 37.139 | 1.00 | 21.15 | H | O |
| ATOM | 2679 | CG2 | THR | 165 | 108.348 | -10.419 | 37.184 | 1.00 | 20.86 | H | C |
| ATOM | 2680 | C | THR | 165 | 108.394 | -13.770 | 35.397 | 1.00 | 33.42 | H | C |
| ATOM | 2681 | O | THR | 165 | 108.028 | -13.717 | 34.227 | 1.00 | 34.44 | H | O |
| ATOM | 2682 | N | SER | 166 | 109.244 | -14.683 | 35.849 | 1.00 | 63.46 | H | N |
| ATOM | 2683 | CA | SER | 166 | 109.804 | -15.702 | 34.973 | 1.00 | 62.93 | H | C |
| ATOM | 2684 | CB | SER | 166 | 110.901 | -16.472 | 35.710 | 1.00 | 37.10 | H | C |
| ATOM | 2685 | OG | SER | 166 | 111.503 | -17.442 | 34.870 | 1.00 | 42.11 | H | O |
| ATOM | 2686 | C | SER | 166 | 108.748 | -16.678 | 34.458 | 1.00 | 60.85 | H | C |
| ATOM | 2687 | O | SER | 166 | 107.955 | -17.226 | 35.227 | 1.00 | 60.31 | H | O |
| ATOM | 2688 | N | GLY | 167 | 108.744 | -16.895 | 33.148 | 1.00 | 58.61 | H | N |
| ATOM | 2689 | CA | GLY | 167 | 107.784 | -17.812 | 32.566 | 1.00 | 55.44 | H | C |
| ATOM | 2690 | C | GLY | 167 | 106.425 | -17.181 | 32.332 | 1.00 | 49.55 | H | C |
| ATOM | 2691 | O | GLY | 167 | 105.462 | -17.878 | 32.010 | 1.00 | 51.52 | H | O |
| ATOM | 2692 | N | VAL | 168 | 106.340 | -15.864 | 32.491 | 1.00 | 12.32 | H | N |
| ATOM | 2693 | CA | VAL | 168 | 105.081 | -15.183 | 32.280 | 1.00 | 12.04 | H | C |
| ATOM | 2694 | CB | VAL | 168 | 104.933 | -13.970 | 33.190 | 1.00 | 2.74 | H | C |
| ATOM | 2695 | CG1 | VAL | 168 | 103.590 | -13.273 | 32.906 | 1.00 | 2.74 | H | C |
| ATOM | 2696 | CG2 | VAL | 168 | 105.070 | -14.398 | 34.630 | 1.00 | 2.83 | H | C |
| ATOM | 2697 | C | VAL | 168 | 104.965 | -14.687 | 30.852 | 1.00 | 11.82 | H | C |
| ATOM | 2698 | O | VAL | 168 | 105.894 | -14.087 | 30.319 | 1.00 | 11.28 | H | O |
| ATOM | 2699 | N | HIS | 169 | 103.807 | -14.931 | 30.253 | 1.00 | 28.24 | H | N |
| ATOM | 2700 | CA | HIS | 169 | 103.518 | -14.512 | 28.891 | 1.00 | 24.96 | H | C |
| ATOM | 2701 | CB | HIS | 169 | 103.566 | -15.695 | 27.924 | 1.00 | 1.87 | H | C |

Fig. 19: A-38

```
ATOM   2702  CG  HIS   169     104.935 -16.209  27.634  1.00   1.87    H     C
ATOM   2703  CD2 HIS   169     105.456 -17.452  27.739  1.00  10.72    H     C
ATOM   2704  ND1 HIS   169     105.935 -15.415  27.114  1.00   4.04    H     N
ATOM   2705  CE1 HIS   169     107.015 -16.147  26.912  1.00  11.56    H     C
ATOM   2706  NE2 HIS   169     106.750 -17.387  27.282  1.00   3.03    H     N
ATOM   2707  C   HIS   169     102.106 -13.934  28.818  1.00  26.88    H     C
ATOM   2708  O   HIS   169     101.143 -14.679  28.610  1.00  27.44    H     O
ATOM   2709  N   THR   170     101.960 -12.628  28.995  1.00  15.52    H     N
ATOM   2710  CA  THR   170     100.637 -12.030  28.885  1.00  14.61    H     C
ATOM   2711  CB  THR   170     100.472 -10.872  29.894  1.00  20.19    H     C
ATOM   2712  OG1 THR   170      99.403 -10.021  29.470  1.00  14.32    H     O
ATOM   2713  CG2 THR   170     101.760 -10.096  30.042  1.00  25.14    H     C
ATOM   2714  C   THR   170     100.487 -11.553  27.433  1.00  15.32    H     C
ATOM   2715  O   THR   170     101.023 -10.532  27.053  1.00  11.65    H     O
ATOM   2716  N   PHE   171      99.762 -12.324  26.630  1.00  23.28    H     N
ATOM   2717  CA  PHE   171      99.587 -12.046  25.206  1.00  17.85    H     C
ATOM   2718  CB  PHE   171      98.695 -13.110  24.554  1.00  15.23    H     C
ATOM   2719  CG  PHE   171      99.138 -14.521  24.806  1.00   7.97    H     C
ATOM   2720  CD1 PHE   171      98.731 -15.195  25.955  1.00   8.65    H     C
ATOM   2721  CD2 PHE   171      99.978 -15.174  23.903  1.00   7.84    H     C
ATOM   2722  CE1 PHE   171      99.153 -16.492  26.202  1.00  17.36    H     C
ATOM   2723  CE2 PHE   171     100.407 -16.473  24.144  1.00  15.22    H     C
ATOM   2724  CZ  PHE   171      99.993 -17.133  25.295  1.00  16.34    H     C
ATOM   2725  C   PHE   171      99.032 -10.692  24.793  1.00  18.20    H     C
ATOM   2726  O   PHE   171      98.344 -10.015  25.552  1.00  23.73    H     O
ATOM   2727  N   PRO   172      99.341 -10.278  23.557  1.00  21.77    H     N
ATOM   2728  CD  PRO   172     100.227 -10.890  22.550  1.00  20.32    H     C
ATOM   2729  CA  PRO   172      98.827  -8.999  23.088  1.00  23.20    H     C
ATOM   2730  CB  PRO   172      99.595  -8.775  21.782  1.00  20.71    H     C
ATOM   2731  CG  PRO   172      99.834 -10.148  21.287  1.00  18.82    H     C
ATOM   2732  C   PRO   172      97.339  -9.235  22.876  1.00  25.11    H     C
ATOM   2733  O   PRO   172      96.916 -10.364  22.645  1.00  23.46    H     O
ATOM   2734  N   ALA   173      96.551  -8.172  22.960  1.00  24.67    H     N
ATOM   2735  CA  ALA   173      95.104  -8.267  22.815  1.00  27.18    H     C
ATOM   2736  CB  ALA   173      94.439  -7.079  23.498  1.00   1.87    H     C
ATOM   2737  C   ALA   173      94.604  -8.379  21.391  1.00  30.18    H     C
ATOM   2738  O   ALA   173      95.304  -8.080  20.426  1.00  32.13    H     O
ATOM   2739  N   VAL   174      93.365  -8.820  21.277  1.00  21.72    H     N
ATOM   2740  CA  VAL   174      92.753  -8.964  19.984  1.00  23.16    H     C
ATOM   2741  CB  VAL   174      92.841 -10.406  19.511  1.00  28.95    H     C
ATOM   2742  CG1 VAL   174      92.103 -10.566  18.201  1.00  32.21    H     C
ATOM   2743  CG2 VAL   174      94.305 -10.797  19.356  1.00  26.32    H     C
ATOM   2744  C   VAL   174      91.302  -8.508  20.058  1.00  25.36    H     C
ATOM   2745  O   VAL   174      90.611  -8.718  21.069  1.00  25.35    H     O
ATOM   2746  N   LEU   175      90.860  -7.856  18.987  1.00  41.55    H     N
ATOM   2747  CA  LEU   175      89.504  -7.338  18.890  1.00  40.23    H     C
ATOM   2748  CB  LEU   175      89.443  -6.276  17.787  1.00  23.29    H     C
ATOM   2749  CG  LEU   175      88.728  -4.928  17.990  1.00  20.94    H     C
ATOM   2750  CD1 LEU   175      88.634  -4.511  19.463  1.00  21.45    H     C
ATOM   2751  CD2 LEU   175      89.518  -3.900  17.186  1.00  22.78    H     C
ATOM   2752  C   LEU   175      88.539  -8.474  18.588  1.00  42.85    H     C
ATOM   2753  O   LEU   175      88.738  -9.233  17.638  1.00  45.50    H     O
ATOM   2754  N   GLN   176      87.500  -8.592  19.407  1.00  41.11    H     N
ATOM   2755  CA  GLN   176      86.514  -9.645  19.228  1.00  42.33    H     C
ATOM   2756  CB  GLN   176      85.852  -9.990  20.564  1.00  38.15    H     C
ATOM   2757  CG  GLN   176      86.817 -10.276  21.703  1.00  37.93    H     C
ATOM   2758  CD  GLN   176      86.109 -10.801  22.939  1.00  36.82    H     C
ATOM   2759  OE1 GLN   176      85.562 -11.899  22.923  1.00  36.67    H     O
ATOM   2760  NE2 GLN   176      86.108 -10.014  24.011  1.00  33.13    H     N
ATOM   2761  C   GLN   176      85.439  -9.207  18.245  1.00  44.39    H     C
ATOM   2762  O   GLN   176      85.274  -8.018  17.969  1.00  34.09    H     O
ATOM   2763  N   SER   177      84.708 -10.182  17.718  1.00  59.83    H     N
ATOM   2764  CA  SER   177      83.624  -9.902  16.790  1.00  58.61    H     C
ATOM   2765  CB  SER   177      82.804 -11.177  16.558  1.00 104.21    H     C
ATOM   2766  OG  SER   177      81.708 -10.945  15.689  1.00 104.01    H     O
ATOM   2767  C   SER   177      82.759  -8.832  17.448  1.00  60.09    H     C
ATOM   2768  O   SER   177      82.169  -7.985  16.778  1.00  62.26    H     O
ATOM   2769  N   SER   178      82.722  -8.877  18.778  1.00  34.26    H     N
ATOM   2770  CA  SER   178      81.942  -7.952  19.596  1.00  32.97    H     C
ATOM   2771  CB  SER   178      81.798  -8.510  21.019  1.00  67.89    H     C
ATOM   2772  OG  SER   178      83.057  -8.636  21.663  1.00  66.22    H     O
ATOM   2773  C   SER   178      82.538  -6.554  19.671  1.00  32.95    H     C
ATOM   2774  O   SER   178      81.921  -5.640  20.210  1.00  35.05    H     O
```

Fig. 19: A-39

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2775 | N | GLY | 179 | 83.738 | -6.382 | 19.135 | 1.00 | 43.45 | H | N |
| ATOM | 2776 | CA | GLY | 179 | 84.357 | -5.072 | 19.191 | 1.00 | 46.81 | H | C |
| ATOM | 2777 | C | GLY | 179 | 84.972 | -4.821 | 20.552 | 1.00 | 50.21 | H | C |
| ATOM | 2778 | O | GLY | 179 | 85.380 | -3.707 | 20.869 | 1.00 | 50.30 | H | O |
| ATOM | 2779 | N | LEU | 180 | 85.020 | -5.862 | 21.369 | 1.00 | 30.24 | H | N |
| ATOM | 2780 | CA | LEU | 180 | 85.620 | -5.749 | 22.686 | 1.00 | 32.27 | H | C |
| ATOM | 2781 | CB | LEU | 180 | 84.706 | -6.380 | 23.730 | 1.00 | 33.41 | H | C |
| ATOM | 2782 | CG | LEU | 180 | 83.485 | -5.524 | 24.054 | 1.00 | 32.78 | H | C |
| ATOM | 2783 | CD1 | LEU | 180 | 82.513 | -6.292 | 24.902 | 1.00 | 27.00 | H | C |
| ATOM | 2784 | CD2 | LEU | 180 | 83.943 | -4.278 | 24.781 | 1.00 | 32.58 | H | C |
| ATOM | 2785 | C | LEU | 180 | 86.974 | -6.442 | 22.672 | 1.00 | 32.86 | H | C |
| ATOM | 2786 | O | LEU | 180 | 87.135 | -7.488 | 22.054 | 1.00 | 36.18 | H | O |
| ATOM | 2787 | N | TYR | 181 | 87.952 | -5.843 | 23.336 | 1.00 | 31.41 | H | N |
| ATOM | 2788 | CA | TYR | 181 | 89.293 | -6.409 | 23.387 | 1.00 | 32.68 | H | C |
| ATOM | 2789 | CB | TYR | 181 | 90.297 | -5.323 | 23.792 | 1.00 | 57.58 | H | C |
| ATOM | 2790 | CG | TYR | 181 | 90.773 | -4.445 | 22.651 | 1.00 | 56.39 | H | C |
| ATOM | 2791 | CD1 | TYR | 181 | 91.591 | -4.961 | 21.647 | 1.00 | 57.58 | H | C |
| ATOM | 2792 | CE1 | TYR | 181 | 92.063 | -4.155 | 20.605 | 1.00 | 57.08 | H | C |
| ATOM | 2793 | CD2 | TYR | 181 | 90.430 | -3.092 | 22.585 | 1.00 | 56.67 | H | C |
| ATOM | 2794 | CE2 | TYR | 181 | 90.899 | -2.273 | 21.543 | 1.00 | 57.48 | H | C |
| ATOM | 2795 | CZ | TYR | 181 | 91.717 | -2.816 | 20.559 | 1.00 | 58.33 | H | C |
| ATOM | 2796 | OH | TYR | 181 | 92.202 | -2.033 | 19.533 | 1.00 | 62.35 | H | O |
| ATOM | 2797 | C | TYR | 181 | 89.361 | -7.573 | 24.375 | 1.00 | 31.73 | H | C |
| ATOM | 2798 | O | TYR | 181 | 88.581 | -7.638 | 25.324 | 1.00 | 32.08 | H | O |
| ATOM | 2799 | N | SER | 182 | 90.287 | -8.499 | 24.149 | 1.00 | 35.13 | H | N |
| ATOM | 2800 | CA | SER | 182 | 90.446 | -9.642 | 25.045 | 1.00 | 32.04 | H | C |
| ATOM | 2801 | CB | SER | 182 | 89.439 | -10.741 | 24.700 | 1.00 | 65.40 | H | C |
| ATOM | 2802 | OG | SER | 182 | 89.612 | -11.868 | 25.543 | 1.00 | 59.63 | H | O |
| ATOM | 2803 | C | SER | 182 | 91.860 | -10.209 | 24.970 | 1.00 | 33.65 | H | C |
| ATOM | 2804 | O | SER | 182 | 92.494 | -10.187 | 23.906 | 1.00 | 37.13 | H | O |
| ATOM | 2805 | N | LEU | 183 | 92.351 | -10.713 | 26.101 | 1.00 | 28.98 | H | N |
| ATOM | 2806 | CA | LEU | 183 | 93.689 | -11.290 | 26.152 | 1.00 | 24.91 | H | C |
| ATOM | 2807 | CB | LEU | 183 | 94.753 | -10.179 | 26.189 | 1.00 | 31.36 | H | C |
| ATOM | 2808 | CG | LEU | 183 | 94.913 | -9.263 | 27.414 | 1.00 | 23.12 | H | C |
| ATOM | 2809 | CD1 | LEU | 183 | 95.475 | -10.014 | 28.625 | 1.00 | 27.02 | H | C |
| ATOM | 2810 | CD2 | LEU | 183 | 95.849 | -8.148 | 27.036 | 1.00 | 19.84 | H | C |
| ATOM | 2811 | C | LEU | 183 | 93.898 | -12.209 | 27.342 | 1.00 | 24.58 | H | C |
| ATOM | 2812 | O | LEU | 183 | 93.179 | -12.135 | 28.326 | 1.00 | 18.76 | H | O |
| ATOM | 2813 | N | SER | 184 | 94.894 | -13.077 | 27.250 | 1.00 | 26.13 | H | N |
| ATOM | 2814 | CA | SER | 184 | 95.205 | -13.967 | 28.357 | 1.00 | 26.65 | H | C |
| ATOM | 2815 | CB | SER | 184 | 95.000 | -15.445 | 27.968 | 1.00 | 16.60 | H | C |
| ATOM | 2816 | OG | SER | 184 | 93.638 | -15.750 | 27.710 | 1.00 | 22.49 | H | O |
| ATOM | 2817 | C | SER | 184 | 96.660 | -13.752 | 28.784 | 1.00 | 22.47 | H | C |
| ATOM | 2818 | O | SER | 184 | 97.546 | -13.511 | 27.953 | 1.00 | 21.27 | H | O |
| ATOM | 2819 | N | SER | 185 | 96.896 | -13.786 | 30.087 | 1.00 | 27.49 | H | N |
| ATOM | 2820 | CA | SER | 185 | 98.251 | -13.670 | 30.575 | 1.00 | 25.55 | H | C |
| ATOM | 2821 | CB | SER | 185 | 98.389 | -12.634 | 31.678 | 1.00 | 27.24 | H | C |
| ATOM | 2822 | OG | SER | 185 | 99.760 | -12.516 | 32.031 | 1.00 | 25.68 | H | O |
| ATOM | 2823 | C | SER | 185 | 98.460 | -15.060 | 31.123 | 1.00 | 23.97 | H | C |
| ATOM | 2824 | O | SER | 185 | 97.652 | -15.551 | 31.912 | 1.00 | 25.28 | H | O |
| ATOM | 2825 | N | VAL | 186 | 99.533 | -15.699 | 30.679 | 1.00 | 29.81 | H | N |
| ATOM | 2826 | CA | VAL | 186 | 99.830 | -17.060 | 31.064 | 1.00 | 29.28 | H | C |
| ATOM | 2827 | CB | VAL | 186 | 99.717 | -17.966 | 29.831 | 1.00 | 20.56 | H | C |
| ATOM | 2828 | CG1 | VAL | 186 | 100.305 | -19.306 | 30.112 | 1.00 | 20.80 | H | C |
| ATOM | 2829 | CG2 | VAL | 186 | 98.253 | -18.121 | 29.446 | 1.00 | 19.74 | H | C |
| ATOM | 2830 | C | VAL | 186 | 101.204 | -17.193 | 31.664 | 1.00 | 30.42 | H | C |
| ATOM | 2831 | O | VAL | 186 | 102.097 | -16.416 | 31.357 | 1.00 | 31.20 | H | O |
| ATOM | 2832 | N | VAL | 187 | 101.359 | -18.179 | 32.540 | 1.00 | 29.47 | H | N |
| ATOM | 2833 | CA | VAL | 187 | 102.645 | -18.457 | 33.178 | 1.00 | 26.42 | H | C |
| ATOM | 2834 | CB | VAL | 187 | 102.739 | -17.797 | 34.586 | 1.00 | 27.93 | H | C |
| ATOM | 2835 | CG1 | VAL | 187 | 101.681 | -18.385 | 35.507 | 1.00 | 26.86 | H | C |
| ATOM | 2836 | CG2 | VAL | 187 | 104.134 | -17.994 | 35.180 | 1.00 | 26.29 | H | C |
| ATOM | 2837 | C | VAL | 187 | 102.842 | -19.975 | 33.309 | 1.00 | 20.75 | H | C |
| ATOM | 2838 | O | VAL | 187 | 101.882 | -20.743 | 33.316 | 1.00 | 22.47 | H | O |
| ATOM | 2839 | N | THR | 188 | 104.098 | -20.397 | 33.377 | 1.00 | 5.29 | H | N |
| ATOM | 2840 | CA | THR | 188 | 104.441 | -21.807 | 33.539 | 1.00 | 7.86 | H | C |
| ATOM | 2841 | CB | THR | 188 | 105.280 | -22.327 | 32.366 | 1.00 | 35.20 | H | C |
| ATOM | 2842 | OG1 | THR | 188 | 106.425 | -21.487 | 32.194 | 1.00 | 33.26 | H | O |
| ATOM | 2843 | CG2 | THR | 188 | 104.453 | -22.337 | 31.078 | 1.00 | 39.96 | H | C |
| ATOM | 2844 | C | THR | 188 | 105.270 | -21.870 | 34.802 | 1.00 | 13.86 | H | C |
| ATOM | 2845 | O | THR | 188 | 106.194 | -21.077 | 34.975 | 1.00 | 18.45 | H | O |
| ATOM | 2846 | N | VAL | 189 | 104.921 | -22.799 | 35.688 | 1.00 | 28.00 | H | N |
| ATOM | 2847 | CA | VAL | 189 | 105.613 | -22.963 | 36.965 | 1.00 | 25.42 | H | C |

Fig. 19: A-40

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2848 | CB | VAL | 189 | 104.755 | -22.412 | 38.137 | 1.00 | 24.28 | H | C |
| ATOM | 2849 | CG1 | VAL | 189 | 104.399 | -20.951 | 37.904 | 1.00 | 17.23 | H | C |
| ATOM | 2850 | CG2 | VAL | 189 | 103.478 | -23.234 | 38.270 | 1.00 | 17.84 | H | C |
| ATOM | 2851 | C | VAL | 189 | 105.875 | -24.439 | 37.242 | 1.00 | 32.15 | H | C |
| ATOM | 2852 | O | VAL | 189 | 105.386 | -25.309 | 36.523 | 1.00 | 35.18 | H | O |
| ATOM | 2853 | N | PRO | 190 | 106.671 | -24.738 | 38.280 | 1.00 | 50.39 | H | N |
| ATOM | 2854 | CD | PRO | 190 | 107.545 | -23.823 | 39.036 | 1.00 | 32.03 | H | C |
| ATOM | 2855 | CA | PRO | 190 | 106.962 | -26.133 | 38.624 | 1.00 | 50.40 | H | C |
| ATOM | 2856 | CB | PRO | 190 | 107.911 | -26.001 | 39.814 | 1.00 | 29.50 | H | C |
| ATOM | 2857 | CG | PRO | 190 | 108.651 | -24.746 | 39.514 | 1.00 | 29.72 | H | C |
| ATOM | 2858 | C | PRO | 190 | 105.650 | -26.801 | 39.018 | 1.00 | 50.46 | H | C |
| ATOM | 2859 | O | PRO | 190 | 104.899 | -26.267 | 39.834 | 1.00 | 48.43 | H | O |
| ATOM | 2860 | N | SER | 191 | 105.357 | -27.953 | 38.436 | 1.00 | 54.29 | H | N |
| ATOM | 2861 | CA | SER | 191 | 104.122 | -28.638 | 38.774 | 1.00 | 60.79 | H | C |
| ATOM | 2862 | CB | SER | 191 | 104.111 | -30.036 | 38.157 | 1.00 | 30.49 | H | C |
| ATOM | 2863 | OG | SER | 191 | 104.076 | -29.980 | 36.740 | 1.00 | 31.07 | H | O |
| ATOM | 2864 | C | SER | 191 | 104.009 | -28.730 | 40.297 | 1.00 | 63.91 | H | C |
| ATOM | 2865 | O | SER | 191 | 102.986 | -28.361 | 40.882 | 1.00 | 66.82 | H | O |
| ATOM | 2866 | N | SER | 192 | 105.084 | -29.201 | 40.924 | 1.00 | 39.50 | H | N |
| ATOM | 2867 | CA | SER | 192 | 105.177 | -29.374 | 42.376 | 1.00 | 40.99 | H | C |
| ATOM | 2868 | CB | SER | 192 | 106.602 | -29.776 | 42.739 | 1.00 | 41.75 | H | C |
| ATOM | 2869 | OG | SER | 192 | 107.475 | -28.675 | 42.565 | 1.00 | 41.65 | H | O |
| ATOM | 2870 | C | SER | 192 | 104.795 | -28.150 | 43.220 | 1.00 | 42.26 | H | C |
| ATOM | 2871 | O | SER | 192 | 104.403 | -28.286 | 44.381 | 1.00 | 48.17 | H | O |
| ATOM | 2872 | N | SER | 193 | 104.923 | -26.960 | 42.645 | 1.00 | 20.64 | H | N |
| ATOM | 2873 | CA | SER | 193 | 104.601 | -25.733 | 43.365 | 1.00 | 22.36 | H | C |
| ATOM | 2874 | CB | SER | 193 | 105.396 | -24.567 | 42.771 | 1.00 | 39.90 | H | C |
| ATOM | 2875 | OG | SER | 193 | 104.973 | -24.284 | 41.447 | 1.00 | 36.65 | H | O |
| ATOM | 2876 | C | SER | 193 | 103.097 | -25.380 | 43.392 | 1.00 | 22.92 | H | C |
| ATOM | 2877 | O | SER | 193 | 102.697 | -24.363 | 43.963 | 1.00 | 25.84 | H | O |
| ATOM | 2878 | N | LEU | 194 | 102.268 | -26.218 | 42.776 | 1.00 | 41.78 | H | N |
| ATOM | 2879 | CA | LEU | 194 | 100.827 | -25.974 | 42.741 | 1.00 | 45.87 | H | C |
| ATOM | 2880 | CB | LEU | 194 | 100.172 | -26.850 | 41.677 | 1.00 | 23.80 | H | C |
| ATOM | 2881 | CG | LEU | 194 | 100.533 | -26.605 | 40.216 | 1.00 | 21.31 | H | C |
| ATOM | 2882 | CD1 | LEU | 194 | 99.975 | -27.739 | 39.377 | 1.00 | 19.27 | H | C |
| ATOM | 2883 | CD2 | LEU | 194 | 99.973 | -25.246 | 39.757 | 1.00 | 15.31 | H | C |
| ATOM | 2884 | C | LEU | 194 | 100.177 | -26.276 | 44.080 | 1.00 | 49.01 | H | C |
| ATOM | 2885 | O | LEU | 194 | 99.209 | -25.623 | 44.478 | 1.00 | 48.38 | H | O |
| ATOM | 2886 | N | GLY | 195 | 100.718 | -27.272 | 44.770 | 1.00 | 65.65 | H | N |
| ATOM | 2887 | CA | GLY | 195 | 100.160 | -27.676 | 46.043 | 1.00 | 68.76 | H | C |
| ATOM | 2888 | C | GLY | 195 | 100.625 | -26.877 | 47.235 | 1.00 | 66.22 | H | C |
| ATOM | 2889 | O | GLY | 195 | 100.051 | -26.992 | 48.314 | 1.00 | 68.30 | H | O |
| ATOM | 2890 | N | THR | 196 | 101.659 | -26.067 | 47.053 | 1.00 | 33.26 | H | N |
| ATOM | 2891 | CA | THR | 196 | 102.175 | -25.265 | 48.155 | 1.00 | 32.73 | H | C |
| ATOM | 2892 | CB | THR | 196 | 103.575 | -25.763 | 48.585 | 1.00 | 30.77 | H | C |
| ATOM | 2893 | OG1 | THR | 196 | 104.489 | -25.676 | 47.478 | 1.00 | 28.63 | H | O |
| ATOM | 2894 | CG2 | THR | 196 | 103.488 | -27.213 | 49.071 | 1.00 | 27.23 | H | C |
| ATOM | 2895 | C | THR | 196 | 102.251 | -23.786 | 47.813 | 1.00 | 35.97 | H | C |
| ATOM | 2896 | O | THR | 196 | 102.179 | -22.933 | 48.695 | 1.00 | 36.72 | H | O |
| ATOM | 2897 | N | GLN | 197 | 102.389 | -23.488 | 46.527 | 1.00 | 53.90 | H | N |
| ATOM | 2898 | CA | GLN | 197 | 102.478 | -22.110 | 46.060 | 1.00 | 54.25 | H | C |
| ATOM | 2899 | CB | GLN | 197 | 103.480 | -22.031 | 44.906 | 1.00 | 42.12 | H | C |
| ATOM | 2900 | CG | GLN | 197 | 104.561 | -20.975 | 45.045 | 1.00 | 45.66 | H | C |
| ATOM | 2901 | CD | GLN | 197 | 104.051 | -19.587 | 44.765 | 1.00 | 49.49 | H | C |
| ATOM | 2902 | OE1 | GLN | 197 | 103.257 | -19.032 | 45.528 | 1.00 | 50.05 | H | O |
| ATOM | 2903 | NE2 | GLN | 197 | 104.500 | -19.013 | 43.656 | 1.00 | 49.01 | H | N |
| ATOM | 2904 | C | GLN | 197 | 101.105 | -21.617 | 45.604 | 1.00 | 52.98 | H | C |
| ATOM | 2905 | O | GLN | 197 | 100.314 | -22.382 | 45.050 | 1.00 | 55.53 | H | O |
| ATOM | 2906 | N | THR | 198 | 100.829 | -20.338 | 45.847 | 1.00 | 30.38 | H | N |
| ATOM | 2907 | CA | THR | 198 | 99.559 | -19.719 | 45.470 | 1.00 | 29.29 | H | C |
| ATOM | 2908 | CB | THR | 198 | 98.922 | -18.970 | 46.677 | 1.00 | 45.77 | H | C |
| ATOM | 2909 | OG1 | THR | 198 | 97.546 | -18.682 | 46.404 | 1.00 | 43.55 | H | O |
| ATOM | 2910 | CG2 | THR | 198 | 99.643 | -17.644 | 46.929 | 1.00 | 47.95 | H | C |
| ATOM | 2911 | C | THR | 198 | 99.811 | -18.719 | 44.338 | 1.00 | 27.94 | H | C |
| ATOM | 2912 | O | THR | 198 | 100.722 | -17.891 | 44.413 | 1.00 | 31.22 | H | O |
| ATOM | 2913 | N | TYR | 199 | 99.008 | -18.789 | 43.285 | 1.00 | 40.84 | H | N |
| ATOM | 2914 | CA | TYR | 199 | 99.191 | -17.874 | 42.168 | 1.00 | 31.26 | H | C |
| ATOM | 2915 | CB | TYR | 199 | 99.402 | -18.681 | 40.880 | 1.00 | 39.46 | H | C |
| ATOM | 2916 | CG | TYR | 199 | 100.677 | -19.496 | 40.904 | 1.00 | 33.83 | H | C |
| ATOM | 2917 | CD1 | TYR | 199 | 101.911 | -18.901 | 40.630 | 1.00 | 31.63 | H | C |
| ATOM | 2918 | CE1 | TYR | 199 | 103.107 | -19.626 | 40.735 | 1.00 | 31.28 | H | C |
| ATOM | 2919 | CD2 | TYR | 199 | 100.662 | -20.847 | 41.282 | 1.00 | 32.94 | H | C |
| ATOM | 2920 | CE2 | TYR | 199 | 101.850 | -21.590 | 41.392 | 1.00 | 33.91 | H | C |

Fig. 19: A-41

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2921 | CZ | TYR | 199 | 103.069 | -20.972 | 41.118 | 1.00 | 33.40 | H | C |
| ATOM | 2922 | OH | TYR | 199 | 104.244 | -21.685 | 41.223 | 1.00 | 37.29 | H | O |
| ATOM | 2923 | C | TYR | 199 | 98.029 | -16.897 | 42.014 | 1.00 | 31.50 | H | C |
| ATOM | 2924 | O | TYR | 199 | 96.876 | -17.302 | 41.913 | 1.00 | 32.18 | H | O |
| ATOM | 2925 | N | ILE | 200 | 98.342 | -15.605 | 42.026 | 1.00 | 38.61 | H | N |
| ATOM | 2926 | CA | ILE | 200 | 97.329 | -14.566 | 41.858 | 1.00 | 39.11 | H | C |
| ATOM | 2927 | CB | ILE | 200 | 97.265 | -13.574 | 43.051 | 1.00 | 27.10 | H | C |
| ATOM | 2928 | CG2 | ILE | 200 | 96.185 | -12.540 | 42.793 | 1.00 | 26.36 | H | C |
| ATOM | 2929 | CG1 | ILE | 200 | 96.978 | -14.301 | 44.363 | 1.00 | 30.59 | H | C |
| ATOM | 2930 | CD1 | ILE | 200 | 98.119 | -15.184 | 44.842 | 1.00 | 36.15 | H | C |
| ATOM | 2931 | C | ILE | 200 | 97.730 | -13.736 | 40.649 | 1.00 | 41.59 | H | C |
| ATOM | 2932 | O | ILE | 200 | 98.916 | -13.517 | 40.415 | 1.00 | 45.01 | H | O |
| ATOM | 2933 | N | CYS | 201 | 96.758 | -13.283 | 39.867 | 1.00 | 30.01 | H | N |
| ATOM | 2934 | CA | CYS | 201 | 97.092 | -12.434 | 38.735 | 1.00 | 27.23 | H | C |
| ATOM | 2935 | C | CYS | 201 | 96.476 | -11.075 | 39.011 | 1.00 | 24.60 | H | C |
| ATOM | 2936 | O | CYS | 201 | 95.307 | -10.967 | 39.386 | 1.00 | 22.36 | H | O |
| ATOM | 2937 | CB | CYS | 201 | 96.577 | -12.997 | 37.394 | 1.00 | 42.80 | H | C |
| ATOM | 2938 | SG | CYS | 201 | 94.784 | -12.909 | 37.090 | 1.00 | 39.16 | H | S |
| ATOM | 2939 | N | ASN | 202 | 97.282 | -10.035 | 38.849 | 1.00 | 26.40 | H | N |
| ATOM | 2940 | CA | ASN | 202 | 96.819 | -8.683 | 39.080 | 1.00 | 32.39 | H | C |
| ATOM | 2941 | CB | ASN | 202 | 97.884 | -7.902 | 39.846 | 1.00 | 36.85 | H | C |
| ATOM | 2942 | CG | ASN | 202 | 98.507 | -8.720 | 40.954 | 1.00 | 39.80 | H | C |
| ATOM | 2943 | OD1 | ASN | 202 | 99.570 | -9.314 | 40.779 | 1.00 | 38.11 | H | O |
| ATOM | 2944 | ND2 | ASN | 202 | 97.837 | -8.776 | 42.097 | 1.00 | 41.02 | H | N |
| ATOM | 2945 | C | ASN | 202 | 96.530 | -8.025 | 37.743 | 1.00 | 36.08 | H | C |
| ATOM | 2946 | O | ASN | 202 | 97.419 | -7.867 | 36.911 | 1.00 | 40.34 | H | O |
| ATOM | 2947 | N | VAL | 203 | 95.273 | -7.668 | 37.533 | 1.00 | 28.99 | H | N |
| ATOM | 2948 | CA | VAL | 203 | 94.868 | -7.017 | 36.295 | 1.00 | 29.18 | H | C |
| ATOM | 2949 | CB | VAL | 203 | 93.691 | -7.781 | 35.624 | 1.00 | 21.70 | H | C |
| ATOM | 2950 | CG1 | VAL | 203 | 93.321 | -7.134 | 34.274 | 1.00 | 17.35 | H | C |
| ATOM | 2951 | CG2 | VAL | 203 | 94.067 | -9.236 | 35.450 | 1.00 | 25.16 | H | C |
| ATOM | 2952 | C | VAL | 203 | 94.443 | -5.580 | 36.615 | 1.00 | 32.31 | H | C |
| ATOM | 2953 | O | VAL | 203 | 93.808 | -5.320 | 37.643 | 1.00 | 27.84 | H | O |
| ATOM | 2954 | N | ASN | 204 | 94.799 | -4.648 | 35.741 | 1.00 | 45.86 | H | N |
| ATOM | 2955 | CA | ASN | 204 | 94.442 | -3.266 | 35.979 | 1.00 | 50.50 | H | C |
| ATOM | 2956 | CB | ASN | 204 | 95.565 | -2.570 | 36.739 | 1.00 | 59.79 | H | C |
| ATOM | 2957 | CG | ASN | 204 | 95.186 | -1.176 | 37.164 | 1.00 | 65.34 | H | C |
| ATOM | 2958 | OD1 | ASN | 204 | 94.801 | -0.347 | 36.338 | 1.00 | 69.10 | H | O |
| ATOM | 2959 | ND2 | ASN | 204 | 95.287 | -0.906 | 38.459 | 1.00 | 65.59 | H | N |
| ATOM | 2960 | C | ASN | 204 | 94.109 | -2.486 | 34.709 | 1.00 | 51.54 | H | C |
| ATOM | 2961 | O | ASN | 204 | 94.985 | -2.164 | 33.905 | 1.00 | 51.77 | H | O |
| ATOM | 2962 | N | HIS | 205 | 92.828 | -2.176 | 34.550 | 1.00 | 30.40 | H | N |
| ATOM | 2963 | CA | HIS | 205 | 92.338 | -1.431 | 33.396 | 1.00 | 29.10 | H | C |
| ATOM | 2964 | CB | HIS | 205 | 90.994 | -1.998 | 32.957 | 1.00 | 20.87 | H | C |
| ATOM | 2965 | CG | HIS | 205 | 90.444 | -1.371 | 31.718 | 1.00 | 25.68 | H | C |
| ATOM | 2966 | CD2 | HIS | 205 | 89.209 | -0.889 | 31.437 | 1.00 | 28.69 | H | C |
| ATOM | 2967 | ND1 | HIS | 205 | 91.165 | -1.282 | 30.548 | 1.00 | 23.44 | H | N |
| ATOM | 2968 | CE1 | HIS | 205 | 90.396 | -0.780 | 29.597 | 1.00 | 25.19 | H | C |
| ATOM | 2969 | NE2 | HIS | 205 | 89.203 | -0.534 | 30.110 | 1.00 | 28.16 | H | N |
| ATOM | 2970 | C | HIS | 205 | 92.157 | 0.022 | 33.793 | 1.00 | 30.12 | H | C |
| ATOM | 2971 | O | HIS | 205 | 91.057 | 0.429 | 34.173 | 1.00 | 28.02 | H | O |
| ATOM | 2972 | N | LYS | 206 | 93.228 | 0.805 | 33.714 | 1.00 | 50.94 | H | N |
| ATOM | 2973 | CA | LYS | 206 | 93.138 | 2.209 | 34.084 | 1.00 | 49.11 | H | C |
| ATOM | 2974 | CB | LYS | 206 | 94.486 | 2.906 | 33.867 | 1.00 | 50.82 | H | C |
| ATOM | 2975 | CG | LYS | 206 | 95.536 | 2.476 | 34.895 | 1.00 | 57.82 | H | C |
| ATOM | 2976 | CD | LYS | 206 | 96.809 | 3.325 | 34.857 | 1.00 | 61.64 | H | C |
| ATOM | 2977 | CE | LYS | 206 | 97.793 | 2.906 | 35.959 | 1.00 | 63.00 | H | C |
| ATOM | 2978 | NZ | LYS | 206 | 99.049 | 3.715 | 35.960 | 1.00 | 66.30 | H | N |
| ATOM | 2979 | C | LYS | 206 | 92.017 | 2.949 | 33.353 | 1.00 | 47.68 | H | C |
| ATOM | 2980 | O | LYS | 206 | 91.318 | 3.765 | 33.955 | 1.00 | 46.73 | H | O |
| ATOM | 2981 | N | PRO | 207 | 91.810 | 2.650 | 32.057 | 1.00 | 33.42 | H | N |
| ATOM | 2982 | CD | PRO | 207 | 92.613 | 1.722 | 31.239 | 1.00 | 21.52 | H | C |
| ATOM | 2983 | CA | PRO | 207 | 90.770 | 3.285 | 31.241 | 1.00 | 34.06 | H | C |
| ATOM | 2984 | CB | PRO | 207 | 90.831 | 2.501 | 29.936 | 1.00 | 21.18 | H | C |
| ATOM | 2985 | CG | PRO | 207 | 92.286 | 2.156 | 29.831 | 1.00 | 24.69 | H | C |
| ATOM | 2986 | C | PRO | 207 | 89.366 | 3.280 | 31.846 | 1.00 | 34.36 | H | C |
| ATOM | 2987 | O | PRO | 207 | 88.452 | 3.927 | 31.311 | 1.00 | 32.31 | H | O |
| ATOM | 2988 | N | SER | 208 | 89.190 | 2.545 | 32.944 | 1.00 | 25.18 | H | N |
| ATOM | 2989 | CA | SER | 208 | 87.893 | 2.481 | 33.628 | 1.00 | 28.11 | H | C |
| ATOM | 2990 | CB | SER | 208 | 87.055 | 1.320 | 33.094 | 1.00 | 29.27 | H | C |
| ATOM | 2991 | OG | SER | 208 | 87.724 | 0.096 | 33.315 | 1.00 | 27.44 | H | O |
| ATOM | 2992 | C | SER | 208 | 88.120 | 2.314 | 35.126 | 1.00 | 31.08 | H | C |
| ATOM | 2993 | O | SER | 208 | 87.266 | 1.789 | 35.846 | 1.00 | 34.78 | H | O |

Fig. 19: A-42

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2994 | N | ASN | 209 | 89.284 | 2.777 | 35.573 | 1.00 | 68.02 | H | N |
| ATOM | 2995 | CA | ASN | 209 | 89.678 | 2.701 | 36.970 | 1.00 | 70.18 | H | C |
| ATOM | 2996 | CB | ASN | 209 | 89.073 | 3.879 | 37.741 | 1.00 | 49.77 | H | C |
| ATOM | 2997 | CG | ASN | 209 | 89.673 | 4.044 | 39.125 | 1.00 | 56.50 | H | C |
| ATOM | 2998 | OD1 | ASN | 209 | 90.885 | 3.963 | 39.301 | 1.00 | 62.08 | H | O |
| ATOM | 2999 | ND2 | ASN | 209 | 88.824 | 4.290 | 40.114 | 1.00 | 57.03 | H | N |
| ATOM | 3000 | C | ASN | 209 | 89.267 | 1.360 | 37.593 | 1.00 | 68.80 | H | C |
| ATOM | 3001 | O | ASN | 209 | 88.708 | 1.304 | 38.690 | 1.00 | 68.05 | H | O |
| ATOM | 3002 | N | THR | 210 | 89.555 | 0.282 | 36.871 | 1.00 | 35.45 | H | N |
| ATOM | 3003 | CA | THR | 210 | 89.246 | -1.061 | 37.322 | 1.00 | 37.08 | H | C |
| ATOM | 3004 | CB | THR | 210 | 88.640 | -1.883 | 36.201 | 1.00 | 55.80 | H | C |
| ATOM | 3005 | OG1 | THR | 210 | 87.416 | -1.273 | 35.787 | 1.00 | 56.14 | H | O |
| ATOM | 3006 | CG2 | THR | 210 | 88.367 | -3.303 | 36.668 | 1.00 | 57.05 | H | C |
| ATOM | 3007 | C | THR | 210 | 90.538 | -1.719 | 37.762 | 1.00 | 36.35 | H | C |
| ATOM | 3008 | O | THR | 210 | 91.613 | -1.388 | 37.266 | 1.00 | 34.79 | H | O |
| ATOM | 3009 | N | LYS | 211 | 90.426 | -2.655 | 38.692 | 1.00 | 33.96 | H | N |
| ATOM | 3010 | CA | LYS | 211 | 91.588 | -3.352 | 39.207 | 1.00 | 34.09 | H | C |
| ATOM | 3011 | CB | LYS | 211 | 92.366 | -2.422 | 40.154 | 1.00 | 52.60 | H | C |
| ATOM | 3012 | CG | LYS | 211 | 93.360 | -3.095 | 41.117 | 1.00 | 57.40 | H | C |
| ATOM | 3013 | CD | LYS | 211 | 94.338 | -4.040 | 40.416 | 1.00 | 62.07 | H | C |
| ATOM | 3014 | CE | LYS | 211 | 95.636 | -4.228 | 41.216 | 1.00 | 64.56 | H | C |
| ATOM | 3015 | NZ | LYS | 211 | 95.432 | -4.548 | 42.660 | 1.00 | 65.70 | H | N |
| ATOM | 3016 | C | LYS | 211 | 91.147 | -4.609 | 39.935 | 1.00 | 32.12 | H | C |
| ATOM | 3017 | O | LYS | 211 | 90.611 | -4.525 | 41.036 | 1.00 | 32.03 | H | O |
| ATOM | 3018 | N | VAL | 212 | 91.357 | -5.772 | 39.322 | 1.00 | 43.02 | H | N |
| ATOM | 3019 | CA | VAL | 212 | 90.971 | -7.017 | 39.973 | 1.00 | 37.80 | H | C |
| ATOM | 3020 | CB | VAL | 212 | 89.728 | -7.685 | 39.308 | 1.00 | 28.95 | H | C |
| ATOM | 3021 | CG1 | VAL | 212 | 88.671 | -6.639 | 39.021 | 1.00 | 26.33 | H | C |
| ATOM | 3022 | CG2 | VAL | 212 | 90.125 | -8.431 | 38.059 | 1.00 | 26.83 | H | C |
| ATOM | 3023 | C | VAL | 212 | 92.086 | -8.042 | 40.020 | 1.00 | 39.84 | H | C |
| ATOM | 3024 | O | VAL | 212 | 92.832 | -8.224 | 39.057 | 1.00 | 39.92 | H | O |
| ATOM | 3025 | N | ASP | 213 | 92.184 | -8.709 | 41.162 | 1.00 | 52.39 | H | N |
| ATOM | 3026 | CA | ASP | 213 | 93.177 | -9.743 | 41.376 | 1.00 | 49.02 | H | C |
| ATOM | 3027 | CB | ASP | 213 | 93.900 | -9.493 | 42.692 | 1.00 | 46.86 | H | C |
| ATOM | 3028 | CG | ASP | 213 | 94.548 | -8.128 | 42.740 | 1.00 | 52.80 | H | C |
| ATOM | 3029 | OD1 | ASP | 213 | 95.420 | -7.852 | 41.887 | 1.00 | 56.11 | H | O |
| ATOM | 3030 | OD2 | ASP | 213 | 94.182 | -7.329 | 43.626 | 1.00 | 57.38 | H | O |
| ATOM | 3031 | C | ASP | 213 | 92.433 | -11.067 | 41.423 | 1.00 | 46.03 | H | C |
| ATOM | 3032 | O | ASP | 213 | 91.537 | -11.248 | 42.236 | 1.00 | 45.16 | H | O |
| ATOM | 3033 | N | LYS | 214 | 92.796 | -11.993 | 40.548 | 1.00 | 33.42 | H | N |
| ATOM | 3034 | CA | LYS | 214 | 92.124 | -13.282 | 40.502 | 1.00 | 29.46 | H | C |
| ATOM | 3035 | CB | LYS | 214 | 91.732 | -13.602 | 39.055 | 0.00 | 52.86 | H | C |
| ATOM | 3036 | CG | LYS | 214 | 90.422 | -14.370 | 38.875 | 0.00 | 47.62 | H | C |
| ATOM | 3037 | CD | LYS | 214 | 90.398 | -15.699 | 39.614 | 0.00 | 43.68 | H | C |
| ATOM | 3038 | CE | LYS | 214 | 89.852 | -15.541 | 41.024 | 0.00 | 41.24 | H | C |
| ATOM | 3039 | NZ | LYS | 214 | 88.452 | -15.037 | 41.021 | 0.00 | 39.27 | H | N |
| ATOM | 3040 | C | LYS | 214 | 93.027 | -14.377 | 41.047 | 1.00 | 29.68 | H | C |
| ATOM | 3041 | O | LYS | 214 | 94.160 | -14.549 | 40.585 | 1.00 | 27.06 | H | O |
| ATOM | 3042 | N | LYS | 215 | 92.533 | -15.103 | 42.045 | 1.00 | 38.49 | H | N |
| ATOM | 3043 | CA | LYS | 215 | 93.289 | -16.207 | 42.617 | 1.00 | 34.59 | H | C |
| ATOM | 3044 | CB | LYS | 215 | 92.788 | -16.531 | 44.032 | 0.00 | 48.10 | H | C |
| ATOM | 3045 | CG | LYS | 215 | 92.812 | -15.343 | 44.987 | 0.00 | 42.43 | H | C |
| ATOM | 3046 | CD | LYS | 215 | 92.403 | -15.737 | 46.401 | 0.00 | 38.17 | H | C |
| ATOM | 3047 | CE | LYS | 215 | 93.458 | -16.597 | 47.089 | 0.00 | 35.48 | H | C |
| ATOM | 3048 | NZ | LYS | 215 | 93.695 | -17.895 | 46.397 | 0.00 | 33.32 | H | N |
| ATOM | 3049 | C | LYS | 215 | 93.042 | -17.391 | 41.675 | 1.00 | 36.50 | H | C |
| ATOM | 3050 | O | LYS | 215 | 91.901 | -17.770 | 41.413 | 1.00 | 38.63 | H | O |
| ATOM | 3051 | N | VAL | 216 | 94.113 | -17.939 | 41.122 | 1.00 | 32.15 | H | N |
| ATOM | 3052 | CA | VAL | 216 | 93.996 | -19.081 | 40.224 | 1.00 | 32.08 | H | C |
| ATOM | 3053 | CB | VAL | 216 | 94.801 | -18.850 | 38.923 | 1.00 | 21.03 | H | C |
| ATOM | 3054 | CG1 | VAL | 216 | 94.435 | -19.912 | 37.880 | 1.00 | 20.14 | H | C |
| ATOM | 3055 | CG2 | VAL | 216 | 94.482 | -17.480 | 38.375 | 1.00 | 18.92 | H | C |
| ATOM | 3056 | C | VAL | 216 | 94.504 | -20.334 | 40.948 | 1.00 | 33.21 | H | C |
| ATOM | 3057 | O | VAL | 216 | 95.696 | -20.441 | 41.248 | 1.00 | 33.32 | H | O |
| ATOM | 3058 | N | GLU | 217 | 93.586 | -21.269 | 41.219 | 1.00 | 45.06 | H | N |
| ATOM | 3059 | CA | GLU | 217 | 93.871 | -22.508 | 41.949 | 1.00 | 48.19 | H | C |
| ATOM | 3060 | CB | GLU | 217 | 93.065 | -22.532 | 43.250 | 1.00 | 91.11 | H | C |
| ATOM | 3061 | CG | GLU | 217 | 93.114 | -21.248 | 44.065 | 1.00 | 95.99 | H | C |
| ATOM | 3062 | CD | GLU | 217 | 91.872 | -21.005 | 44.901 | 1.00 | 101.94 | H | C |
| ATOM | 3063 | OE1 | GLU | 217 | 90.757 | -21.353 | 44.453 | 1.00 | 105.02 | H | O |
| ATOM | 3064 | OE2 | GLU | 217 | 92.013 | -20.475 | 46.029 | 1.00 | 105.37 | H | O |
| ATOM | 3065 | C | GLU | 217 | 93.426 | -23.720 | 41.109 | 1.00 | 48.96 | H | C |
| ATOM | 3066 | O | GLU | 217 | 92.500 | -23.643 | 40.332 | 1.00 | 51.24 | H | O |

Fig. 19: A-43

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 3067 | N | PRO | 218 | 94.078 | -24.870 | 41.265 | 1.00 | 42.53 | H | N |
| ATOM | 3068 | CD | PRO | 218 | 95.339 | -25.074 | 41.993 | 1.00 | 48.02 | H | C |
| ATOM | 3069 | CA | PRO | 218 | 93.711 | -26.079 | 40.509 | 1.00 | 40.69 | H | C |
| ATOM | 3070 | CB | PRO | 218 | 94.962 | -26.924 | 40.609 | 1.00 | 42.70 | H | C |
| ATOM | 3071 | CG | PRO | 218 | 95.482 | -26.557 | 41.957 | 1.00 | 44.19 | H | C |
| ATOM | 3072 | C | PRO | 218 | 92.544 | -26.782 | 41.183 | 1.00 | 41.85 | H | C |
| ATOM | 3073 | O | PRO | 218 | 92.513 | -26.844 | 42.403 | 1.00 | 45.36 | H | O |
| ATOM | 3074 | N | LYS | 219 | 91.638 | -27.354 | 40.396 | 1.00 | 112.06 | H | N |
| ATOM | 3075 | CA | LYS | 219 | 90.475 | -28.045 | 40.934 | 1.00 | 111.92 | H | C |
| ATOM | 3076 | CB | LYS | 219 | 89.635 | -28.618 | 39.794 | 0.00 | 52.93 | H | C |
| ATOM | 3077 | CG | LYS | 219 | 89.522 | -27.658 | 38.654 | 0.00 | 47.21 | H | C |
| ATOM | 3078 | CD | LYS | 219 | 88.205 | -27.801 | 37.948 | 0.00 | 42.71 | H | C |
| ATOM | 3079 | CE | LYS | 219 | 88.174 | -26.793 | 36.845 | 0.00 | 39.84 | H | C |
| ATOM | 3080 | NZ | LYS | 219 | 86.847 | -26.599 | 36.249 | 0.00 | 37.57 | H | N |
| ATOM | 3081 | C | LYS | 219 | 90.867 | -29.169 | 41.892 | 1.00 | 116.73 | H | C |
| ATOM | 3082 | O | LYS | 219 | 90.330 | -29.223 | 43.021 | 1.00 | 116.18 | H | O |
| ATOM | 3083 | OXT | LYS | 219 | 91.705 | -30.007 | 41.503 | 1.00 | 36.39 | H | O |
| ATOM | 3084 | CB | ILE | 2 | 109.298 | 10.543 | -2.157 | 1.00 | 31.85 | L | C |
| ATOM | 3085 | CG2 | ILE | 2 | 110.285 | 9.382 | -2.130 | 1.00 | 31.85 | L | C |
| ATOM | 3086 | CG1 | ILE | 2 | 109.803 | 11.664 | -3.069 | 1.00 | 31.85 | L | C |
| ATOM | 3087 | CD1 | ILE | 2 | 111.143 | 12.240 | -2.656 | 1.00 | 31.85 | L | C |
| ATOM | 3088 | C | ILE | 2 | 107.518 | 8.858 | -1.778 | 1.00 | 41.66 | L | C |
| ATOM | 3089 | O | ILE | 2 | 107.155 | 9.019 | -0.613 | 1.00 | 41.66 | L | O |
| ATOM | 3090 | N | ILE | 2 | 106.898 | 11.133 | -2.646 | 1.00 | 41.66 | L | N |
| ATOM | 3091 | CA | ILE | 2 | 107.922 | 10.043 | -2.648 | 1.00 | 41.66 | L | C |
| ATOM | 3092 | N | GLN | 3 | 107.597 | 7.665 | -2.361 | 1.00 | 28.81 | L | N |
| ATOM | 3093 | CA | GLN | 3 | 107.244 | 6.433 | -1.669 | 1.00 | 28.81 | L | C |
| ATOM | 3094 | CB | GLN | 3 | 106.206 | 5.677 | -2.484 | 1.00 | 56.92 | L | C |
| ATOM | 3095 | CG | GLN | 3 | 105.708 | 4.412 | -1.837 | 1.00 | 56.92 | L | C |
| ATOM | 3096 | CD | GLN | 3 | 104.579 | 3.778 | -2.622 | 1.00 | 56.92 | L | C |
| ATOM | 3097 | OE1 | GLN | 3 | 104.124 | 2.681 | -2.298 | 1.00 | 56.92 | L | O |
| ATOM | 3098 | NE2 | GLN | 3 | 104.116 | 4.469 | -3.661 | 1.00 | 56.92 | L | N |
| ATOM | 3099 | C | GLN | 3 | 108.482 | 5.557 | -1.428 | 1.00 | 28.81 | L | C |
| ATOM | 3100 | O | GLN | 3 | 109.297 | 5.322 | -2.327 | 1.00 | 28.81 | L | O |
| ATOM | 3101 | N | LEU | 4 | 108.615 | 5.088 | -0.195 | 1.00 | 39.62 | L | N |
| ATOM | 3102 | CA | LEU | 4 | 109.744 | 4.260 | 0.198 | 1.00 | 39.62 | L | C |
| ATOM | 3103 | CB | LEU | 4 | 110.377 | 4.820 | 1.469 | 1.00 | 19.64 | L | C |
| ATOM | 3104 | CG | LEU | 4 | 111.546 | 5.792 | 1.348 | 1.00 | 19.64 | L | C |
| ATOM | 3105 | CD1 | LEU | 4 | 111.407 | 6.643 | 0.092 | 1.00 | 19.64 | L | C |
| ATOM | 3106 | CD2 | LEU | 4 | 111.614 | 6.640 | 2.617 | 1.00 | 19.64 | L | C |
| ATOM | 3107 | C | LEU | 4 | 109.323 | 2.823 | 0.445 | 1.00 | 39.62 | L | C |
| ATOM | 3108 | O | LEU | 4 | 108.470 | 2.548 | 1.289 | 1.00 | 39.62 | L | O |
| ATOM | 3109 | N | THR | 5 | 109.935 | 1.903 | -0.289 | 1.00 | 16.92 | L | N |
| ATOM | 3110 | CA | THR | 5 | 109.634 | 0.485 | -0.152 | 1.00 | 16.92 | L | C |
| ATOM | 3111 | CB | THR | 5 | 108.945 | -0.038 | -1.437 | 1.00 | 21.45 | L | C |
| ATOM | 3112 | OG1 | THR | 5 | 109.307 | -1.402 | -1.651 | 1.00 | 21.45 | L | O |
| ATOM | 3113 | CG2 | THR | 5 | 109.324 | 0.802 | -2.641 | 1.00 | 21.45 | L | C |
| ATOM | 3114 | C | THR | 5 | 110.908 | -0.312 | 0.186 | 1.00 | 16.92 | L | C |
| ATOM | 3115 | O | THR | 5 | 111.849 | -0.382 | -0.601 | 1.00 | 16.92 | L | O |
| ATOM | 3116 | N | GLN | 6 | 110.919 | -0.880 | 1.391 | 1.00 | 17.69 | L | N |
| ATOM | 3117 | CA | GLN | 6 | 112.040 | -1.661 | 1.933 | 1.00 | 17.69 | L | C |
| ATOM | 3118 | CB | GLN | 6 | 112.078 | -1.544 | 3.468 | 1.00 | 15.96 | L | C |
| ATOM | 3119 | CG | GLN | 6 | 111.898 | -0.138 | 4.014 | 1.00 | 15.96 | L | C |
| ATOM | 3120 | CD | GLN | 6 | 112.007 | -0.060 | 5.535 | 1.00 | 15.96 | L | C |
| ATOM | 3121 | OE1 | GLN | 6 | 111.626 | 0.944 | 6.139 | 1.00 | 15.96 | L | O |
| ATOM | 3122 | NE2 | GLN | 6 | 112.541 | -1.115 | 6.158 | 1.00 | 15.96 | L | N |
| ATOM | 3123 | C | GLN | 6 | 111.962 | -3.143 | 1.588 | 1.00 | 17.69 | L | C |
| ATOM | 3124 | O | GLN | 6 | 110.882 | -3.675 | 1.352 | 1.00 | 17.69 | L | O |
| ATOM | 3125 | N | SER | 7 | 113.107 | -3.814 | 1.595 | 1.00 | 44.56 | L | N |
| ATOM | 3126 | CA | SER | 7 | 113.148 | -5.238 | 1.293 | 1.00 | 44.56 | L | C |
| ATOM | 3127 | CB | SER | 7 | 113.109 | -5.470 | -0.214 | 1.00 | 33.18 | L | C |
| ATOM | 3128 | OG | SER | 7 | 114.194 | -4.813 | -0.837 | 1.00 | 33.18 | L | O |
| ATOM | 3129 | C | SER | 7 | 114.394 | -5.898 | 1.855 | 1.00 | 44.56 | L | C |
| ATOM | 3130 | O | SER | 7 | 115.480 | -5.328 | 1.811 | 1.00 | 44.56 | L | O |
| ATOM | 3131 | N | PRO | 8 | 114.246 | -7.107 | 2.415 | 1.00 | 19.10 | L | N |
| ATOM | 3132 | CD | PRO | 8 | 115.292 | -7.921 | 3.063 | 1.00 | 16.76 | L | C |
| ATOM | 3133 | CA | PRO | 8 | 112.945 | -7.771 | 2.494 | 1.00 | 19.10 | L | C |
| ATOM | 3134 | CB | PRO | 8 | 113.303 | -9.161 | 3.004 | 1.00 | 16.76 | L | C |
| ATOM | 3135 | CG | PRO | 8 | 114.481 | -8.882 | 3.905 | 1.00 | 16.76 | L | C |
| ATOM | 3136 | C | PRO | 8 | 112.068 | -7.023 | 3.479 | 1.00 | 19.10 | L | C |
| ATOM | 3137 | O | PRO | 8 | 112.517 | -6.069 | 4.125 | 1.00 | 19.10 | L | O |
| ATOM | 3138 | N | SER | 9 | 110.822 | -7.460 | 3.589 | 1.00 | 12.41 | L | N |
| ATOM | 3139 | CA | SER | 9 | 109.885 | -6.851 | 4.516 | 1.00 | 12.41 | L | C |

Fig. 19: A-44

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 3140 | CB | SER | 9 | 108.466 | -7.059 | 4.023 | 1.00 | 25.43 | L | C |
| ATOM | 3141 | OG | SER | 9 | 108.345 | -6.555 | 2.707 | 1.00 | 25.43 | L | O |
| ATOM | 3142 | C | SER | 9 | 110.083 | -7.558 | 5.837 | 1.00 | 12.41 | L | C |
| ATOM | 3143 | O | SER | 9 | 109.904 | -6.983 | 6.904 | 1.00 | 12.41 | L | O |
| ATOM | 3144 | N | SER | 10 | 110.492 | -8.817 | 5.745 | 1.00 | 33.63 | L | N |
| ATOM | 3145 | CA | SER | 10 | 110.720 | -9.645 | 6.910 | 1.00 | 33.63 | L | C |
| ATOM | 3146 | CB | SER | 10 | 109.490 | -10.517 | 7.144 | 1.00 | 43.13 | L | C |
| ATOM | 3147 | OG | SER | 10 | 109.614 | -11.248 | 8.338 | 1.00 | 43.13 | L | O |
| ATOM | 3148 | C | SER | 10 | 111.942 | -10.504 | 6.624 | 1.00 | 33.63 | L | C |
| ATOM | 3149 | O | SER | 10 | 112.226 | -10.814 | 5.470 | 1.00 | 33.63 | L | O |
| ATOM | 3150 | N | LEU | 11 | 112.677 | -10.880 | 7.666 | 1.00 | 38.19 | L | N |
| ATOM | 3151 | CA | LEU | 11 | 113.867 | -11.709 | 7.484 | 1.00 | 38.19 | L | C |
| ATOM | 3152 | CB | LEU | 11 | 115.020 | -10.880 | 6.894 | 1.00 | 33.64 | L | C |
| ATOM | 3153 | CG | LEU | 11 | 115.721 | -9.849 | 7.793 | 1.00 | 33.64 | L | C |
| ATOM | 3154 | CD1 | LEU | 11 | 116.757 | -10.532 | 8.667 | 1.00 | 33.64 | L | C |
| ATOM | 3155 | CD2 | LEU | 11 | 116.401 | -8.807 | 6.927 | 1.00 | 33.64 | L | C |
| ATOM | 3156 | C | LEU | 11 | 114.319 | -12.335 | 8.792 | 1.00 | 38.19 | L | C |
| ATOM | 3157 | O | LEU | 11 | 114.365 | -11.672 | 9.829 | 1.00 | 38.19 | L | O |
| ATOM | 3158 | N | SER | 12 | 114.661 | -13.616 | 8.736 | 1.00 | 42.98 | L | N |
| ATOM | 3159 | CA | SER | 12 | 115.128 | -14.320 | 9.916 | 1.00 | 42.98 | L | C |
| ATOM | 3160 | CB | SER | 12 | 114.334 | -15.612 | 10.103 | 1.00 | 67.78 | L | C |
| ATOM | 3161 | OG | SER | 12 | 114.474 | -16.092 | 11.426 | 1.00 | 67.78 | L | O |
| ATOM | 3162 | C | SER | 12 | 116.611 | -14.628 | 9.738 | 1.00 | 42.98 | L | C |
| ATOM | 3163 | O | SER | 12 | 117.031 | -15.118 | 8.697 | 1.00 | 42.98 | L | O |
| ATOM | 3164 | N | ALA | 13 | 117.407 | -14.320 | 10.749 | 1.00 | 25.03 | L | N |
| ATOM | 3165 | CA | ALA | 13 | 118.836 | -14.575 | 10.667 | 1.00 | 25.03 | L | C |
| ATOM | 3166 | CB | ALA | 13 | 119.556 | -13.340 | 10.124 | 1.00 | 41.64 | L | C |
| ATOM | 3167 | C | ALA | 13 | 119.390 | -14.952 | 12.037 | 1.00 | 25.03 | L | C |
| ATOM | 3168 | O | ALA | 13 | 118.829 | -14.571 | 13.067 | 1.00 | 25.03 | L | O |
| ATOM | 3169 | N | SER | 14 | 120.493 | -15.701 | 12.045 | 1.00 | 32.48 | L | N |
| ATOM | 3170 | CA | SER | 14 | 121.111 | -16.132 | 13.294 | 1.00 | 32.48 | L | C |
| ATOM | 3171 | CB | SER | 14 | 121.594 | -17.569 | 13.160 | 1.00 | 77.12 | L | C |
| ATOM | 3172 | OG | SER | 14 | 122.348 | -17.721 | 11.975 | 1.00 | 77.12 | L | O |
| ATOM | 3173 | C | SER | 14 | 122.269 | -15.231 | 13.691 | 1.00 | 32.48 | L | C |
| ATOM | 3174 | O | SER | 14 | 122.893 | -14.595 | 12.841 | 1.00 | 32.48 | L | O |
| ATOM | 3175 | N | VAL | 15 | 122.545 | -15.166 | 14.988 | 1.00 | 47.29 | L | N |
| ATOM | 3176 | CA | VAL | 15 | 123.637 | -14.336 | 15.470 | 1.00 | 47.29 | L | C |
| ATOM | 3177 | CB | VAL | 15 | 123.996 | -14.657 | 16.937 | 1.00 | 53.16 | L | C |
| ATOM | 3178 | CG1 | VAL | 15 | 123.121 | -13.847 | 17.881 | 1.00 | 53.16 | L | C |
| ATOM | 3179 | CG2 | VAL | 15 | 123.808 | -16.148 | 17.198 | 1.00 | 53.16 | L | C |
| ATOM | 3180 | C | VAL | 15 | 124.858 | -14.575 | 14.606 | 1.00 | 47.29 | L | C |
| ATOM | 3181 | O | VAL | 15 | 125.164 | -15.712 | 14.250 | 1.00 | 47.29 | L | O |
| ATOM | 3182 | N | GLY | 16 | 125.537 | -13.495 | 14.247 | 1.00 | 32.44 | L | N |
| ATOM | 3183 | CA | GLY | 16 | 126.728 | -13.615 | 13.431 | 1.00 | 32.44 | L | C |
| ATOM | 3184 | C | GLY | 16 | 126.506 | -13.463 | 11.945 | 1.00 | 32.44 | L | C |
| ATOM | 3185 | O | GLY | 16 | 127.467 | -13.306 | 11.191 | 1.00 | 32.44 | L | O |
| ATOM | 3186 | N | ASP | 17 | 125.255 | -13.524 | 11.510 | 1.00 | 32.03 | L | N |
| ATOM | 3187 | CA | ASP | 17 | 124.959 | -13.367 | 10.092 | 1.00 | 32.03 | L | C |
| ATOM | 3188 | CB | ASP | 17 | 123.533 | -13.814 | 9.788 | 1.00 | 55.01 | L | C |
| ATOM | 3189 | CG | ASP | 17 | 123.344 | -15.291 | 9.961 | 1.00 | 55.01 | L | C |
| ATOM | 3190 | OD1 | ASP | 17 | 122.211 | -15.771 | 9.739 | 1.00 | 55.01 | L | O |
| ATOM | 3191 | OD2 | ASP | 17 | 124.331 | -15.965 | 10.320 | 1.00 | 55.01 | L | O |
| ATOM | 3192 | C | ASP | 17 | 125.109 | -11.905 | 9.677 | 1.00 | 32.03 | L | C |
| ATOM | 3193 | O | ASP | 17 | 125.041 | -10.997 | 10.517 | 1.00 | 32.03 | L | O |
| ATOM | 3194 | N | ARG | 18 | 125.324 | -11.680 | 8.385 | 1.00 | 40.86 | L | N |
| ATOM | 3195 | CA | ARG | 18 | 125.447 | -10.325 | 7.875 | 1.00 | 40.86 | L | C |
| ATOM | 3196 | CB | ARG | 18 | 126.587 | -10.231 | 6.865 | 1.00 | 78.37 | L | C |
| ATOM | 3197 | CG | ARG | 18 | 126.790 | -8.842 | 6.293 | 1.00 | 78.37 | L | C |
| ATOM | 3198 | CD | ARG | 18 | 128.223 | -8.662 | 5.812 | 1.00 | 78.37 | L | C |
| ATOM | 3199 | NE | ARG | 18 | 128.413 | -7.408 | 5.087 | 1.00 | 78.37 | L | N |
| ATOM | 3200 | CZ | ARG | 18 | 127.841 | -7.131 | 3.918 | 1.00 | 78.37 | L | C |
| ATOM | 3201 | NH1 | ARG | 18 | 127.042 | -8.021 | 3.336 | 1.00 | 78.37 | L | N |
| ATOM | 3202 | NH2 | ARG | 18 | 128.064 | -5.960 | 3.334 | 1.00 | 78.37 | L | N |
| ATOM | 3203 | C | ARG | 18 | 124.116 | -9.986 | 7.220 | 1.00 | 40.86 | L | C |
| ATOM | 3204 | O | ARG | 18 | 123.690 | -10.656 | 6.284 | 1.00 | 40.86 | L | O |
| ATOM | 3205 | N | VAL | 19 | 123.455 | -8.948 | 7.721 | 1.00 | 26.42 | L | N |
| ATOM | 3206 | CA | VAL | 19 | 122.157 | -8.549 | 7.193 | 1.00 | 26.42 | L | C |
| ATOM | 3207 | CB | VAL | 19 | 121.154 | -8.426 | 8.335 | 1.00 | 32.94 | L | C |
| ATOM | 3208 | CG1 | VAL | 19 | 119.768 | -8.214 | 7.783 | 1.00 | 32.94 | L | C |
| ATOM | 3209 | CG2 | VAL | 19 | 121.204 | -9.678 | 9.194 | 1.00 | 32.94 | L | C |
| ATOM | 3210 | C | VAL | 19 | 122.200 | -7.235 | 6.420 | 1.00 | 26.42 | L | C |
| ATOM | 3211 | O | VAL | 19 | 122.902 | -6.306 | 6.798 | 1.00 | 26.42 | L | O |
| ATOM | 3212 | N | THR | 20 | 121.443 | -7.160 | 5.333 | 1.00 | 42.24 | L | N |

Fig. 19: A-45

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 3213 | CA | THR | 20 | 121.408 | -5.950 | 4.519 | 1.00 | 42.24 | L | C |
| ATOM | 3214 | CB | THR | 20 | 122.310 | -6.097 | 3.289 | 1.00 | 29.90 | L | C |
| ATOM | 3215 | OG1 | THR | 20 | 123.680 | -6.127 | 3.714 | 1.00 | 29.90 | L | O |
| ATOM | 3216 | CG2 | THR | 20 | 122.099 | -4.944 | 2.326 | 1.00 | 29.90 | L | C |
| ATOM | 3217 | C | THR | 20 | 120.008 | -5.582 | 4.050 | 1.00 | 42.24 | L | C |
| ATOM | 3218 | O | THR | 20 | 119.477 | -6.202 | 3.127 | 1.00 | 42.24 | L | O |
| ATOM | 3219 | N | ILE | 21 | 119.418 | -4.568 | 4.683 | 1.00 | 13.95 | L | N |
| ATOM | 3220 | CA | ILE | 21 | 118.077 | -4.114 | 4.326 | 1.00 | 13.95 | L | C |
| ATOM | 3221 | CB | ILE | 21 | 117.349 | -3.486 | 5.541 | 1.00 | 24.11 | L | C |
| ATOM | 3222 | CG2 | ILE | 21 | 115.892 | -3.176 | 5.186 | 1.00 | 24.11 | L | C |
| ATOM | 3223 | CG1 | ILE | 21 | 117.390 | -4.457 | 6.720 | 1.00 | 24.11 | L | C |
| ATOM | 3224 | CD1 | ILE | 21 | 116.709 | -3.936 | 7.960 | 1.00 | 24.11 | L | C |
| ATOM | 3225 | C | ILE | 21 | 118.180 | -3.081 | 3.217 | 1.00 | 13.95 | L | C |
| ATOM | 3226 | O | ILE | 21 | 119.036 | -2.208 | 3.251 | 1.00 | 13.95 | L | O |
| ATOM | 3227 | N | THR | 22 | 117.305 | -3.190 | 2.230 | 1.00 | 27.07 | L | N |
| ATOM | 3228 | CA | THR | 22 | 117.304 | -2.266 | 1.107 | 1.00 | 27.07 | L | C |
| ATOM | 3229 | CB | THR | 22 | 117.335 | -3.022 | -0.239 | 1.00 | 29.03 | L | C |
| ATOM | 3230 | OG1 | THR | 22 | 118.613 | -3.642 | -0.404 | 1.00 | 29.03 | L | O |
| ATOM | 3231 | CG2 | THR | 22 | 117.084 | -2.084 | -1.391 | 1.00 | 29.03 | L | C |
| ATOM | 3232 | C | THR | 22 | 116.067 | -1.385 | 1.123 | 1.00 | 27.07 | L | C |
| ATOM | 3233 | O | THR | 22 | 114.951 | -1.871 | 1.313 | 1.00 | 27.07 | L | O |
| ATOM | 3234 | N | CYS | 23 | 116.281 | -0.089 | 0.916 | 1.00 | 32.83 | L | N |
| ATOM | 3235 | CA | CYS | 23 | 115.203 | 0.896 | 0.882 | 1.00 | 32.83 | L | C |
| ATOM | 3236 | C | CYS | 23 | 115.259 | 1.546 | -0.489 | 1.00 | 32.83 | L | C |
| ATOM | 3237 | O | CYS | 23 | 116.250 | 2.187 | -0.837 | 1.00 | 32.83 | L | O |
| ATOM | 3238 | CB | CYS | 23 | 115.424 | 1.947 | 1.973 | 1.00 | 18.66 | L | C |
| ATOM | 3239 | SG | CYS | 23 | 114.216 | 3.310 | 2.141 | 1.00 | 18.66 | L | S |
| ATOM | 3240 | N | SER | 24 | 114.199 | 1.355 | -1.268 | 1.00 | 11.34 | L | N |
| ATOM | 3241 | CA | SER | 24 | 114.110 | 1.924 | -2.612 | 1.00 | 11.34 | L | C |
| ATOM | 3242 | CB | SER | 24 | 113.696 | 0.853 | -3.614 | 1.00 | 28.67 | L | C |
| ATOM | 3243 | OG | SER | 24 | 114.642 | -0.190 | -3.632 | 1.00 | 28.67 | L | O |
| ATOM | 3244 | C | SER | 24 | 113.096 | 3.058 | -2.641 | 1.00 | 11.34 | L | C |
| ATOM | 3245 | O | SER | 24 | 111.971 | 2.910 | -2.154 | 1.00 | 11.34 | L | O |
| ATOM | 3246 | N | ALA | 25 | 113.496 | 4.186 | -3.217 | 1.00 | 32.05 | L | N |
| ATOM | 3247 | CA | ALA | 25 | 112.617 | 5.343 | -3.286 | 1.00 | 32.05 | L | C |
| ATOM | 3248 | CB | ALA | 25 | 113.312 | 6.567 | -2.707 | 1.00 | 44.86 | L | C |
| ATOM | 3249 | C | ALA | 25 | 112.139 | 5.633 | -4.699 | 1.00 | 32.05 | L | C |
| ATOM | 3250 | O | ALA | 25 | 112.918 | 5.619 | -5.658 | 1.00 | 32.05 | L | O |
| ATOM | 3251 | N | SER | 26 | 110.839 | 5.901 | -4.803 | 1.00 | 26.80 | L | N |
| ATOM | 3252 | CA | SER | 26 | 110.179 | 6.204 | -6.070 | 1.00 | 26.80 | L | C |
| ATOM | 3253 | CB | SER | 26 | 108.717 | 6.572 | -5.814 | 1.00 | 23.33 | L | C |
| ATOM | 3254 | OG | SER | 26 | 108.617 | 7.713 | -4.984 | 1.00 | 23.33 | L | O |
| ATOM | 3255 | C | SER | 26 | 110.866 | 7.338 | -6.813 | 1.00 | 26.80 | L | C |
| ATOM | 3256 | O | SER | 26 | 110.814 | 7.404 | -8.032 | 1.00 | 26.80 | L | O |
| ATOM | 3257 | N | SER | 27 | 111.496 | 8.234 | -6.066 | 1.00 | 22.71 | L | N |
| ATOM | 3258 | CA | SER | 27 | 112.210 | 9.363 | -6.644 | 1.00 | 22.71 | L | C |
| ATOM | 3259 | CB | SER | 27 | 111.439 | 10.661 | -6.406 | 1.00 | 47.74 | L | C |
| ATOM | 3260 | OG | SER | 27 | 110.105 | 10.552 | -6.862 | 1.00 | 47.74 | L | O |
| ATOM | 3261 | C | SER | 27 | 113.547 | 9.438 | -5.934 | 1.00 | 22.71 | L | C |
| ATOM | 3262 | O | SER | 27 | 113.666 | 8.982 | -4.805 | 1.00 | 22.71 | L | O |
| ATOM | 3263 | N | SER | 28 | 114.555 | 10.004 | -6.586 | 1.00 | 37.73 | L | N |
| ATOM | 3264 | CA | SER | 28 | 115.874 | 10.121 | -5.972 | 1.00 | 37.73 | L | C |
| ATOM | 3265 | CB | SER | 28 | 116.890 | 10.583 | -7.010 | 1.00 | 36.75 | L | C |
| ATOM | 3266 | OG | SER | 28 | 116.486 | 11.818 | -7.573 | 1.00 | 36.75 | L | O |
| ATOM | 3267 | C | SER | 28 | 115.846 | 11.106 | -4.804 | 1.00 | 37.73 | L | C |
| ATOM | 3268 | O | SER | 28 | 115.043 | 12.038 | -4.775 | 1.00 | 37.73 | L | O |
| ATOM | 3269 | N | VAL | 29 | 116.726 | 10.890 | -3.838 | 1.00 | 35.34 | L | N |
| ATOM | 3270 | CA | VAL | 29 | 116.807 | 11.753 | -2.669 | 1.00 | 35.34 | L | C |
| ATOM | 3271 | CB | VAL | 29 | 116.002 | 11.154 | -1.484 | 1.00 | 39.96 | L | C |
| ATOM | 3272 | CG1 | VAL | 29 | 114.521 | 11.097 | -1.842 | 1.00 | 39.96 | L | C |
| ATOM | 3273 | CG2 | VAL | 29 | 116.506 | 9.755 | -1.147 | 1.00 | 39.96 | L | C |
| ATOM | 3274 | C | VAL | 29 | 118.277 | 11.895 | -2.289 | 1.00 | 35.34 | L | C |
| ATOM | 3275 | O | VAL | 29 | 119.076 | 11.001 | -2.571 | 1.00 | 35.34 | L | O |
| ATOM | 3276 | N | ASN | 30 | 118.641 | 13.007 | -1.658 | 1.00 | 55.44 | L | N |
| ATOM | 3277 | CA | ASN | 30 | 120.033 | 13.236 | -1.278 | 1.00 | 55.44 | L | C |
| ATOM | 3278 | CB | ASN | 30 | 120.252 | 14.722 | -0.974 | 1.00 | 66.75 | L | C |
| ATOM | 3279 | CG | ASN | 30 | 119.176 | 15.292 | -0.071 | 1.00 | 66.75 | L | C |
| ATOM | 3280 | OD1 | ASN | 30 | 118.006 | 15.359 | -0.453 | 1.00 | 66.75 | L | O |
| ATOM | 3281 | ND2 | ASN | 30 | 119.561 | 15.694 | 1.138 | 1.00 | 66.75 | L | N |
| ATOM | 3282 | C | ASN | 30 | 120.510 | 12.386 | -0.095 | 1.00 | 55.44 | L | C |
| ATOM | 3283 | O | ASN | 30 | 121.705 | 12.099 | 0.033 | 1.00 | 55.44 | L | O |
| ATOM | 3284 | N | HIS | 31 | 119.586 | 11.985 | 0.770 | 1.00 | 34.66 | L | N |
| ATOM | 3285 | CA | HIS | 31 | 119.947 | 11.172 | 1.923 | 1.00 | 34.66 | L | C |

Fig. 19: A-46

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 3286 | CB | HIS | 31 | 120.290 | 12.049 | 3.132 | 1.00 | 51.96 | L | C |
| ATOM | 3287 | CG | HIS | 31 | 121.623 | 12.725 | 3.042 | 1.00 | 51.96 | L | C |
| ATOM | 3288 | CD2 | HIS | 31 | 122.763 | 12.534 | 3.744 | 1.00 | 51.96 | L | C |
| ATOM | 3289 | ND1 | HIS | 31 | 121.879 | 13.763 | 2.172 | 1.00 | 51.96 | L | N |
| ATOM | 3290 | CE1 | HIS | 31 | 123.118 | 14.186 | 2.345 | 1.00 | 51.96 | L | C |
| ATOM | 3291 | NE2 | HIS | 31 | 123.676 | 13.457 | 3.294 | 1.00 | 51.96 | L | N |
| ATOM | 3292 | C | HIS | 31 | 118.811 | 10.241 | 2.316 | 1.00 | 34.66 | L | C |
| ATOM | 3293 | O | HIS | 31 | 117.736 | 10.267 | 1.707 | 1.00 | 34.66 | L | O |
| ATOM | 3294 | N | MET | 32 | 119.070 | 9.415 | 3.332 | 1.00 | 24.85 | L | N |
| ATOM | 3295 | CA | MET | 32 | 118.081 | 8.489 | 3.864 | 1.00 | 24.85 | L | C |
| ATOM | 3296 | CB | MET | 32 | 118.189 | 7.126 | 3.187 | 1.00 | 22.87 | L | C |
| ATOM | 3297 | CG | MET | 32 | 116.961 | 6.226 | 3.394 | 1.00 | 22.87 | L | C |
| ATOM | 3298 | SD | MET | 32 | 115.381 | 6.922 | 2.757 | 1.00 | 22.87 | L | S |
| ATOM | 3299 | CE | MET | 32 | 115.727 | 7.028 | 1.012 | 1.00 | 22.87 | L | C |
| ATOM | 3300 | C | MET | 32 | 118.316 | 8.340 | 5.360 | 1.00 | 24.85 | L | C |
| ATOM | 3301 | O | MET | 32 | 119.454 | 8.377 | 5.831 | 1.00 | 24.85 | L | O |
| ATOM | 3302 | N | PHE | 33 | 117.244 | 8.180 | 6.118 | 1.00 | 7.47 | L | N |
| ATOM | 3303 | CA | PHE | 33 | 117.391 | 8.029 | 7.554 | 1.00 | 7.47 | L | C |
| ATOM | 3304 | CB | PHE | 33 | 116.693 | 9.171 | 8.285 | 1.00 | 11.22 | L | C |
| ATOM | 3305 | CG | PHE | 33 | 117.205 | 10.533 | 7.901 | 1.00 | 11.22 | L | C |
| ATOM | 3306 | CD1 | PHE | 33 | 116.901 | 11.078 | 6.652 | 1.00 | 11.22 | L | C |
| ATOM | 3307 | CD2 | PHE | 33 | 118.017 | 11.259 | 8.776 | 1.00 | 11.22 | L | C |
| ATOM | 3308 | CE1 | PHE | 33 | 117.399 | 12.325 | 6.275 | 1.00 | 11.22 | L | C |
| ATOM | 3309 | CE2 | PHE | 33 | 118.519 | 12.501 | 8.407 | 1.00 | 11.22 | L | C |
| ATOM | 3310 | CZ | PHE | 33 | 118.207 | 13.035 | 7.149 | 1.00 | 11.22 | L | C |
| ATOM | 3311 | C | PHE | 33 | 116.817 | 6.702 | 7.994 | 1.00 | 7.47 | L | C |
| ATOM | 3312 | O | PHE | 33 | 115.959 | 6.150 | 7.320 | 1.00 | 7.47 | L | O |
| ATOM | 3313 | N | TRP | 34 | 117.301 | 6.186 | 9.118 | 1.00 | 15.67 | L | N |
| ATOM | 3314 | CA | TRP | 34 | 116.815 | 4.912 | 9.618 | 1.00 | 15.67 | L | C |
| ATOM | 3315 | CB | TRP | 34 | 117.859 | 3.818 | 9.414 | 1.00 | 16.49 | L | C |
| ATOM | 3316 | CG | TRP | 34 | 118.217 | 3.590 | 7.992 | 1.00 | 16.49 | L | C |
| ATOM | 3317 | CD2 | TRP | 34 | 117.671 | 2.592 | 7.123 | 1.00 | 16.49 | L | C |
| ATOM | 3318 | CE2 | TRP | 34 | 118.315 | 2.732 | 5.872 | 1.00 | 16.49 | L | C |
| ATOM | 3319 | CE3 | TRP | 34 | 116.702 | 1.596 | 7.279 | 1.00 | 16.49 | L | C |
| ATOM | 3320 | CD1 | TRP | 34 | 119.137 | 4.278 | 7.259 | 1.00 | 16.49 | L | C |
| ATOM | 3321 | NE1 | TRP | 34 | 119.205 | 3.767 | 5.984 | 1.00 | 16.49 | L | N |
| ATOM | 3322 | CZ2 | TRP | 34 | 118.024 | 1.914 | 4.782 | 1.00 | 16.49 | L | C |
| ATOM | 3323 | CZ3 | TRP | 34 | 116.409 | 0.780 | 6.194 | 1.00 | 16.49 | L | C |
| ATOM | 3324 | CH2 | TRP | 34 | 117.069 | 0.945 | 4.960 | 1.00 | 16.49 | L | C |
| ATOM | 3325 | C | TRP | 34 | 116.459 | 4.960 | 11.086 | 1.00 | 15.67 | L | C |
| ATOM | 3326 | O | TRP | 34 | 117.149 | 5.593 | 11.882 | 1.00 | 15.67 | L | O |
| ATOM | 3327 | N | TYR | 35 | 115.370 | 4.288 | 11.437 | 1.00 | 19.71 | L | N |
| ATOM | 3328 | CA | TYR | 35 | 114.939 | 4.229 | 12.820 | 1.00 | 19.71 | L | C |
| ATOM | 3329 | CB | TYR | 35 | 113.591 | 4.922 | 13.007 | 1.00 | 25.75 | L | C |
| ATOM | 3330 | CG | TYR | 35 | 113.623 | 6.381 | 12.621 | 1.00 | 25.75 | L | C |
| ATOM | 3331 | CD1 | TYR | 35 | 113.255 | 6.790 | 11.344 | 1.00 | 25.75 | L | C |
| ATOM | 3332 | CE1 | TYR | 35 | 113.310 | 8.124 | 10.980 | 1.00 | 25.75 | L | C |
| ATOM | 3333 | CD2 | TYR | 35 | 114.052 | 7.353 | 13.527 | 1.00 | 25.75 | L | C |
| ATOM | 3334 | CE2 | TYR | 35 | 114.110 | 8.685 | 13.173 | 1.00 | 25.75 | L | C |
| ATOM | 3335 | CZ | TYR | 35 | 113.737 | 9.064 | 11.899 | 1.00 | 25.75 | L | C |
| ATOM | 3336 | OH | TYR | 35 | 113.776 | 10.384 | 11.540 | 1.00 | 25.75 | L | O |
| ATOM | 3337 | C | TYR | 35 | 114.821 | 2.781 | 13.207 | 1.00 | 19.71 | L | C |
| ATOM | 3338 | O | TYR | 35 | 114.508 | 1.937 | 12.373 | 1.00 | 19.71 | L | O |
| ATOM | 3339 | N | GLN | 36 | 115.100 | 2.491 | 14.468 | 1.00 | 30.18 | L | N |
| ATOM | 3340 | CA | GLN | 36 | 114.987 | 1.136 | 14.964 | 1.00 | 30.18 | L | C |
| ATOM | 3341 | CB | GLN | 36 | 116.292 | 0.659 | 15.597 | 1.00 | 33.56 | L | C |
| ATOM | 3342 | CG | GLN | 36 | 116.109 | -0.625 | 16.387 | 1.00 | 33.56 | L | C |
| ATOM | 3343 | CD | GLN | 36 | 117.154 | -0.806 | 17.464 | 1.00 | 33.56 | L | C |
| ATOM | 3344 | OE1 | GLN | 36 | 118.296 | -1.161 | 17.179 | 1.00 | 33.56 | L | O |
| ATOM | 3345 | NE2 | GLN | 36 | 116.770 | -0.550 | 18.716 | 1.00 | 33.56 | L | N |
| ATOM | 3346 | C | GLN | 36 | 113.902 | 1.124 | 16.017 | 1.00 | 30.18 | L | C |
| ATOM | 3347 | O | GLN | 36 | 113.986 | 1.852 | 17.008 | 1.00 | 30.18 | L | O |
| ATOM | 3348 | N | GLN | 37 | 112.877 | 0.311 | 15.803 | 1.00 | 31.84 | L | N |
| ATOM | 3349 | CA | GLN | 37 | 111.811 | 0.209 | 16.778 | 1.00 | 31.84 | L | C |
| ATOM | 3350 | CB | GLN | 37 | 110.467 | 0.599 | 16.162 | 1.00 | 26.28 | L | C |
| ATOM | 3351 | CG | GLN | 37 | 109.335 | 0.494 | 17.165 | 1.00 | 26.28 | L | C |
| ATOM | 3352 | CD | GLN | 37 | 108.003 | 0.979 | 16.632 | 1.00 | 26.28 | L | C |
| ATOM | 3353 | OE1 | GLN | 37 | 107.573 | 0.597 | 15.537 | 1.00 | 26.28 | L | O |
| ATOM | 3354 | NE2 | GLN | 37 | 107.328 | 1.819 | 17.417 | 1.00 | 26.28 | L | N |
| ATOM | 3355 | C | GLN | 37 | 111.729 | -1.201 | 17.360 | 1.00 | 31.84 | L | C |
| ATOM | 3356 | O | GLN | 37 | 111.571 | -2.189 | 16.637 | 1.00 | 31.84 | L | O |
| ATOM | 3357 | N | LYS | 38 | 111.861 | -1.285 | 18.676 | 1.00 | 33.78 | L | N |
| ATOM | 3358 | CA | LYS | 38 | 111.776 | -2.561 | 19.366 | 1.00 | 33.78 | L | C |

Fig. 19: A-47

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 3359 | CB | LYS | 38 | 112.784 | -2.618 | 20.519 | 1.00 | 38.31 | L | C |
| ATOM | 3360 | CG | LYS | 38 | 114.209 | -2.306 | 20.094 | 1.00 | 38.31 | L | C |
| ATOM | 3361 | CD | LYS | 38 | 115.224 | -2.552 | 21.207 | 1.00 | 38.31 | L | C |
| ATOM | 3362 | CE | LYS | 38 | 115.494 | -4.034 | 21.402 | 1.00 | 38.31 | L | C |
| ATOM | 3363 | NZ | LYS | 38 | 115.954 | -4.720 | 20.154 | 1.00 | 38.31 | L | N |
| ATOM | 3364 | C | LYS | 38 | 110.346 | -2.671 | 19.889 | 1.00 | 33.78 | L | C |
| ATOM | 3365 | O | LYS | 38 | 109.770 | -1.690 | 20.354 | 1.00 | 33.78 | L | O |
| ATOM | 3366 | N | PRO | 39 | 109.757 | -3.873 | 19.818 | 1.00 | 36.51 | L | N |
| ATOM | 3367 | CD | PRO | 39 | 110.419 | -5.128 | 19.422 | 1.00 | 56.09 | L | C |
| ATOM | 3368 | CA | PRO | 39 | 108.389 | -4.139 | 20.271 | 1.00 | 36.51 | L | C |
| ATOM | 3369 | CB | PRO | 39 | 108.376 | -5.652 | 20.409 | 1.00 | 56.09 | L | C |
| ATOM | 3370 | CG | PRO | 39 | 109.254 | -6.072 | 19.283 | 1.00 | 56.09 | L | C |
| ATOM | 3371 | C | PRO | 39 | 107.976 | -3.434 | 21.559 | 1.00 | 36.51 | L | C |
| ATOM | 3372 | O | PRO | 39 | 108.664 | -3.523 | 22.573 | 1.00 | 36.51 | L | O |
| ATOM | 3373 | N | GLY | 40 | 106.846 | -2.735 | 21.503 | 1.00 | 29.94 | L | N |
| ATOM | 3374 | CA | GLY | 40 | 106.330 | -2.036 | 22.667 | 1.00 | 29.94 | L | C |
| ATOM | 3375 | C | GLY | 40 | 107.025 | -0.738 | 23.034 | 1.00 | 29.94 | L | C |
| ATOM | 3376 | O | GLY | 40 | 106.669 | -0.119 | 24.037 | 1.00 | 29.94 | L | O |
| ATOM | 3377 | N | LYS | 41 | 108.019 | -0.332 | 22.243 | 1.00 | 32.57 | L | N |
| ATOM | 3378 | CA | LYS | 41 | 108.754 | 0.903 | 22.503 | 1.00 | 32.57 | L | C |
| ATOM | 3379 | CB | LYS | 41 | 110.231 | 0.611 | 22.804 | 1.00 | 82.45 | L | C |
| ATOM | 3380 | CG | LYS | 41 | 110.466 | -0.251 | 24.040 | 1.00 | 82.45 | L | C |
| ATOM | 3381 | CD | LYS | 41 | 111.905 | -0.157 | 24.579 | 1.00 | 82.45 | L | C |
| ATOM | 3382 | CE | LYS | 41 | 112.977 | -0.603 | 23.575 | 1.00 | 82.45 | L | C |
| ATOM | 3383 | NZ | LYS | 41 | 113.257 | 0.396 | 22.496 | 1.00 | 82.45 | L | N |
| ATOM | 3384 | C | LYS | 41 | 108.656 | 1.860 | 21.319 | 1.00 | 32.57 | L | C |
| ATOM | 3385 | O | LYS | 41 | 108.243 | 1.480 | 20.227 | 1.00 | 32.57 | L | O |
| ATOM | 3386 | N | ALA | 42 | 109.029 | 3.112 | 21.547 | 1.00 | 30.66 | L | N |
| ATOM | 3387 | CA | ALA | 42 | 108.990 | 4.126 | 20.502 | 1.00 | 30.66 | L | C |
| ATOM | 3388 | CB | ALA | 42 | 108.980 | 5.513 | 21.129 | 1.00 | 32.87 | L | C |
| ATOM | 3389 | C | ALA | 42 | 110.209 | 3.973 | 19.606 | 1.00 | 30.66 | L | C |
| ATOM | 3390 | O | ALA | 42 | 111.235 | 3.436 | 20.028 | 1.00 | 30.66 | L | O |
| ATOM | 3391 | N | PRO | 43 | 110.112 | 4.435 | 18.351 | 1.00 | 23.79 | L | N |
| ATOM | 3392 | CD | PRO | 43 | 108.939 | 4.976 | 17.647 | 1.00 | 7.10 | L | C |
| ATOM | 3393 | CA | PRO | 43 | 111.248 | 4.323 | 17.440 | 1.00 | 23.79 | L | C |
| ATOM | 3394 | CB | PRO | 43 | 110.727 | 4.980 | 16.170 | 1.00 | 7.10 | L | C |
| ATOM | 3395 | CG | PRO | 43 | 109.275 | 4.677 | 16.212 | 1.00 | 7.10 | L | C |
| ATOM | 3396 | C | PRO | 43 | 112.476 | 5.042 | 18.007 | 1.00 | 23.79 | L | C |
| ATOM | 3397 | O | PRO | 43 | 112.359 | 5.903 | 18.877 | 1.00 | 23.79 | L | O |
| ATOM | 3398 | N | LYS | 44 | 113.652 | 4.678 | 17.514 | 1.00 | 26.42 | L | N |
| ATOM | 3399 | CA | LYS | 44 | 114.888 | 5.283 | 17.972 | 1.00 | 26.42 | L | C |
| ATOM | 3400 | CB | LYS | 44 | 115.656 | 4.289 | 18.843 | 1.00 | 45.11 | L | C |
| ATOM | 3401 | CG | LYS | 44 | 115.840 | 4.724 | 20.288 | 1.00 | 45.11 | L | C |
| ATOM | 3402 | CD | LYS | 44 | 116.535 | 3.651 | 21.131 | 1.00 | 45.11 | L | C |
| ATOM | 3403 | CE | LYS | 44 | 115.656 | 2.400 | 21.338 | 1.00 | 45.11 | L | C |
| ATOM | 3404 | NZ | LYS | 44 | 115.359 | 1.613 | 20.087 | 1.00 | 45.11 | L | N |
| ATOM | 3405 | C | LYS | 44 | 115.741 | 5.673 | 16.767 | 1.00 | 26.42 | L | C |
| ATOM | 3406 | O | LYS | 44 | 115.898 | 4.888 | 15.829 | 1.00 | 26.42 | L | O |
| ATOM | 3407 | N | PRO | 45 | 116.287 | 6.902 | 16.764 | 1.00 | 19.50 | L | N |
| ATOM | 3408 | CD | PRO | 45 | 116.146 | 7.943 | 17.794 | 1.00 | 7.61 | L | C |
| ATOM | 3409 | CA | PRO | 45 | 117.132 | 7.362 | 15.649 | 1.00 | 19.50 | L | C |
| ATOM | 3410 | CB | PRO | 45 | 117.638 | 8.720 | 16.120 | 1.00 | 7.61 | L | C |
| ATOM | 3411 | CG | PRO | 45 | 116.547 | 9.180 | 17.041 | 1.00 | 7.61 | L | C |
| ATOM | 3412 | C | PRO | 45 | 118.273 | 6.367 | 15.542 | 1.00 | 19.50 | L | C |
| ATOM | 3413 | O | PRO | 45 | 118.925 | 6.082 | 16.549 | 1.00 | 19.50 | L | O |
| ATOM | 3414 | N | TRP | 46 | 118.521 | 5.848 | 14.342 | 1.00 | 23.41 | L | N |
| ATOM | 3415 | CA | TRP | 46 | 119.581 | 4.861 | 14.158 | 1.00 | 23.41 | L | C |
| ATOM | 3416 | CB | TRP | 46 | 118.980 | 3.559 | 13.643 | 1.00 | 20.77 | L | C |
| ATOM | 3417 | CG | TRP | 46 | 119.662 | 2.382 | 14.178 | 1.00 | 20.77 | L | C |
| ATOM | 3418 | CD2 | TRP | 46 | 119.738 | 2.007 | 15.554 | 1.00 | 20.77 | L | C |
| ATOM | 3419 | CE2 | TRP | 46 | 120.509 | 0.829 | 15.624 | 1.00 | 20.77 | L | C |
| ATOM | 3420 | CE3 | TRP | 46 | 119.229 | 2.554 | 16.737 | 1.00 | 20.77 | L | C |
| ATOM | 3421 | CD1 | TRP | 46 | 120.365 | 1.446 | 13.481 | 1.00 | 20.77 | L | C |
| ATOM | 3422 | NE1 | TRP | 46 | 120.879 | 0.504 | 14.345 | 1.00 | 20.77 | L | N |
| ATOM | 3423 | CZ2 | TRP | 46 | 120.786 | 0.191 | 16.834 | 1.00 | 20.77 | L | C |
| ATOM | 3424 | CZ3 | TRP | 46 | 119.505 | 1.918 | 17.938 | 1.00 | 20.77 | L | C |
| ATOM | 3425 | CH2 | TRP | 46 | 120.276 | 0.750 | 17.977 | 1.00 | 20.77 | L | C |
| ATOM | 3426 | C | TRP | 46 | 120.691 | 5.302 | 13.209 | 1.00 | 23.41 | L | C |
| ATOM | 3427 | O | TRP | 46 | 121.871 | 5.174 | 13.507 | 1.00 | 23.41 | L | O |
| ATOM | 3428 | N | ILE | 47 | 120.306 | 5.806 | 12.048 | 1.00 | 21.62 | L | N |
| ATOM | 3429 | CA | ILE | 47 | 121.275 | 6.248 | 11.073 | 1.00 | 21.62 | L | C |
| ATOM | 3430 | CB | ILE | 47 | 121.515 | 5.160 | 10.008 | 1.00 | 12.16 | L | C |
| ATOM | 3431 | CG2 | ILE | 47 | 122.473 | 5.668 | 8.929 | 1.00 | 12.16 | L | C |

Fig. 19: A-48

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 3432 | CG1 | ILE | 47 | 122.067 | 3.902 | 10.670 | 1.00 | 12.16 | L | C |
| ATOM | 3433 | CD1 | ILE | 47 | 122.301 | 2.746 | 9.686 | 1.00 | 12.16 | L | C |
| ATOM | 3434 | C | ILE | 47 | 120.694 | 7.482 | 10.408 | 1.00 | 21.62 | L | C |
| ATOM | 3435 | O | ILE | 47 | 119.600 | 7.424 | 9.840 | 1.00 | 21.62 | L | O |
| ATOM | 3436 | N | TYR | 48 | 121.408 | 8.603 | 10.510 | 1.00 | 27.63 | L | N |
| ATOM | 3437 | CA | TYR | 48 | 120.961 | 9.842 | 9.887 | 1.00 | 27.63 | L | C |
| ATOM | 3438 | CB | TYR | 48 | 120.899 | 10.992 | 10.892 | 1.00 | 47.89 | L | C |
| ATOM | 3439 | CG | TYR | 48 | 122.206 | 11.318 | 11.564 | 1.00 | 47.89 | L | C |
| ATOM | 3440 | CD1 | TYR | 48 | 122.762 | 10.454 | 12.502 | 1.00 | 47.89 | L | C |
| ATOM | 3441 | CE1 | TYR | 48 | 123.961 | 10.766 | 13.143 | 1.00 | 47.89 | L | C |
| ATOM | 3442 | CD2 | TYR | 48 | 122.881 | 12.503 | 11.277 | 1.00 | 47.89 | L | C |
| ATOM | 3443 | CE2 | TYR | 48 | 124.078 | 12.827 | 11.907 | 1.00 | 47.89 | L | C |
| ATOM | 3444 | CZ | TYR | 48 | 124.617 | 11.957 | 12.843 | 1.00 | 47.89 | L | C |
| ATOM | 3445 | OH | TYR | 48 | 125.803 | 12.269 | 13.483 | 1.00 | 47.89 | L | O |
| ATOM | 3446 | C | TYR | 48 | 121.922 | 10.181 | 8.766 | 1.00 | 27.63 | L | C |
| ATOM | 3447 | O | TYR | 48 | 122.992 | 9.575 | 8.646 | 1.00 | 27.63 | L | O |
| ATOM | 3448 | N | LEU | 49 | 121.535 | 11.150 | 7.948 | 1.00 | 28.95 | L | N |
| ATOM | 3449 | CA | LEU | 49 | 122.344 | 11.550 | 6.811 | 1.00 | 28.95 | L | C |
| ATOM | 3450 | CB | LEU | 49 | 123.421 | 12.568 | 7.232 | 1.00 | 11.18 | L | C |
| ATOM | 3451 | CG | LEU | 49 | 123.051 | 14.040 | 7.473 | 1.00 | 11.18 | L | C |
| ATOM | 3452 | CD1 | LEU | 49 | 122.174 | 14.552 | 6.344 | 1.00 | 11.18 | L | C |
| ATOM | 3453 | CD2 | LEU | 49 | 122.333 | 14.178 | 8.780 | 1.00 | 11.18 | L | C |
| ATOM | 3454 | C | LEU | 49 | 122.997 | 10.350 | 6.117 | 1.00 | 28.95 | L | C |
| ATOM | 3455 | O | LEU | 49 | 124.204 | 10.323 | 5.920 | 1.00 | 28.95 | L | O |
| ATOM | 3456 | N | THR | 50 | 122.192 | 9.351 | 5.777 | 1.00 | 29.56 | L | N |
| ATOM | 3457 | CA | THR | 50 | 122.666 | 8.165 | 5.072 | 1.00 | 29.56 | L | C |
| ATOM | 3458 | CB | THR | 50 | 123.352 | 8.566 | 3.770 | 1.00 | 23.05 | L | C |
| ATOM | 3459 | OG1 | THR | 50 | 122.490 | 9.434 | 3.040 | 1.00 | 23.05 | L | O |
| ATOM | 3460 | CG2 | THR | 50 | 123.647 | 7.335 | 2.923 | 1.00 | 23.05 | L | C |
| ATOM | 3461 | C | THR | 50 | 123.582 | 7.152 | 5.767 | 1.00 | 29.56 | L | C |
| ATOM | 3462 | O | THR | 50 | 123.229 | 5.976 | 5.888 | 1.00 | 29.56 | L | O |
| ATOM | 3463 | N | SER | 51 | 124.757 | 7.586 | 6.203 | 1.00 | 25.90 | L | N |
| ATOM | 3464 | CA | SER | 51 | 125.697 | 6.670 | 6.839 | 1.00 | 25.90 | L | C |
| ATOM | 3465 | CB | SER | 51 | 126.976 | 6.594 | 6.003 | 1.00 | 41.07 | L | C |
| ATOM | 3466 | OG | SER | 51 | 127.467 | 7.893 | 5.715 | 1.00 | 41.07 | L | O |
| ATOM | 3467 | C | SER | 51 | 126.049 | 6.998 | 8.287 | 1.00 | 25.90 | L | C |
| ATOM | 3468 | O | SER | 51 | 126.578 | 6.160 | 9.015 | 1.00 | 25.90 | L | O |
| ATOM | 3469 | N | ASN | 52 | 125.749 | 8.211 | 8.712 | 1.00 | 36.32 | L | N |
| ATOM | 3470 | CA | ASN | 52 | 126.050 | 8.615 | 10.075 | 1.00 | 36.32 | L | C |
| ATOM | 3471 | CB | ASN | 52 | 125.741 | 10.092 | 10.247 | 1.00 | 35.00 | L | C |
| ATOM | 3472 | CG | ASN | 52 | 126.708 | 10.954 | 9.499 | 1.00 | 35.00 | L | C |
| ATOM | 3473 | OD1 | ASN | 52 | 127.881 | 11.022 | 9.857 | 1.00 | 35.00 | L | O |
| ATOM | 3474 | ND2 | ASN | 52 | 126.236 | 11.608 | 8.439 | 1.00 | 35.00 | L | N |
| ATOM | 3475 | C | ASN | 52 | 125.288 | 7.815 | 11.109 | 1.00 | 36.32 | L | C |
| ATOM | 3476 | O | ASN | 52 | 124.059 | 7.766 | 11.078 | 1.00 | 36.32 | L | O |
| ATOM | 3477 | N | LEU | 53 | 126.018 | 7.190 | 12.027 | 1.00 | 27.25 | L | N |
| ATOM | 3478 | CA | LEU | 53 | 125.387 | 6.408 | 13.080 | 1.00 | 27.25 | L | C |
| ATOM | 3479 | CB | LEU | 53 | 126.355 | 5.366 | 13.631 | 1.00 | 36.82 | L | C |
| ATOM | 3480 | CG | LEU | 53 | 126.949 | 4.324 | 12.682 | 1.00 | 36.82 | L | C |
| ATOM | 3481 | CD1 | LEU | 53 | 127.640 | 3.266 | 13.531 | 1.00 | 36.82 | L | C |
| ATOM | 3482 | CD2 | LEU | 53 | 125.876 | 3.674 | 11.822 | 1.00 | 36.82 | L | C |
| ATOM | 3483 | C | LEU | 53 | 124.938 | 7.312 | 14.219 | 1.00 | 27.25 | L | C |
| ATOM | 3484 | O | LEU | 53 | 125.643 | 8.241 | 14.581 | 1.00 | 27.25 | L | O |
| ATOM | 3485 | N | ALA | 54 | 123.763 | 7.043 | 14.779 | 1.00 | 46.43 | L | N |
| ATOM | 3486 | CA | ALA | 54 | 123.251 | 7.827 | 15.897 | 1.00 | 46.43 | L | C |
| ATOM | 3487 | CB | ALA | 54 | 121.938 | 7.272 | 16.373 | 1.00 | 9.56 | L | C |
| ATOM | 3488 | C | ALA | 54 | 124.267 | 7.728 | 17.008 | 1.00 | 46.43 | L | C |
| ATOM | 3489 | O | ALA | 54 | 125.380 | 7.254 | 16.794 | 1.00 | 46.43 | L | O |
| ATOM | 3490 | N | SER | 55 | 123.891 | 8.140 | 18.208 | 1.00 | 82.41 | L | N |
| ATOM | 3491 | CA | SER | 55 | 124.847 | 8.081 | 19.290 | 1.00 | 82.41 | L | C |
| ATOM | 3492 | CB | SER | 55 | 124.439 | 9.036 | 20.406 | 1.00 | 85.12 | L | C |
| ATOM | 3493 | OG | SER | 55 | 125.561 | 9.342 | 21.215 | 1.00 | 85.12 | L | O |
| ATOM | 3494 | C | SER | 55 | 125.049 | 6.675 | 19.850 | 1.00 | 82.41 | L | C |
| ATOM | 3495 | O | SER | 55 | 126.187 | 6.226 | 20.004 | 1.00 | 82.41 | L | O |
| ATOM | 3496 | N | GLY | 56 | 123.957 | 5.970 | 20.137 | 1.00 | 57.94 | L | N |
| ATOM | 3497 | CA | GLY | 56 | 124.074 | 4.632 | 20.701 | 1.00 | 57.94 | L | C |
| ATOM | 3498 | C | GLY | 56 | 124.408 | 3.486 | 19.758 | 1.00 | 57.94 | L | C |
| ATOM | 3499 | O | GLY | 56 | 125.101 | 2.545 | 20.136 | 1.00 | 57.94 | L | O |
| ATOM | 3500 | N | VAL | 57 | 123.914 | 3.562 | 18.530 | 1.00 | 69.56 | L | N |
| ATOM | 3501 | CA | VAL | 57 | 124.131 | 2.519 | 17.530 | 1.00 | 69.56 | L | C |
| ATOM | 3502 | CB | VAL | 57 | 123.809 | 3.053 | 16.108 | 1.00 | 49.85 | L | C |
| ATOM | 3503 | CG1 | VAL | 57 | 123.682 | 1.898 | 15.128 | 1.00 | 49.85 | L | C |
| ATOM | 3504 | CG2 | VAL | 57 | 122.529 | 3.875 | 16.139 | 1.00 | 49.85 | L | C |

Fig. 19: A-49

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 3505 | C | VAL | 57 | 125.544 | 1.929 | 17.513 | 1.00 | 69.56 | L | C |
| ATOM | 3506 | O | VAL | 57 | 126.515 | 2.637 | 17.244 | 1.00 | 69.56 | L | O |
| ATOM | 3507 | N | PRO | 58 | 125.674 | 0.618 | 17.799 | 1.00 | 24.22 | L | N |
| ATOM | 3508 | CD | PRO | 58 | 124.609 | -0.342 | 18.141 | 1.00 | 44.23 | L | C |
| ATOM | 3509 | CA | PRO | 58 | 126.978 | -0.046 | 17.802 | 1.00 | 24.22 | L | C |
| ATOM | 3510 | CB | PRO | 58 | 126.638 | -1.472 | 18.237 | 1.00 | 44.23 | L | C |
| ATOM | 3511 | CG | PRO | 58 | 125.244 | -1.653 | 17.772 | 1.00 | 44.23 | L | C |
| ATOM | 3512 | C | PRO | 58 | 127.609 | 0.017 | 16.415 | 1.00 | 24.22 | L | C |
| ATOM | 3513 | O | PRO | 58 | 126.903 | -0.083 | 15.400 | 1.00 | 24.22 | L | O |
| ATOM | 3514 | N | SER | 59 | 128.935 | 0.174 | 16.381 | 1.00 | 54.17 | L | N |
| ATOM | 3515 | CA | SER | 59 | 129.691 | 0.295 | 15.134 | 1.00 | 54.17 | L | C |
| ATOM | 3516 | CB | SER | 59 | 131.184 | 0.489 | 15.438 | 1.00 | 118.98 | L | C |
| ATOM | 3517 | OG | SER | 59 | 131.729 | -0.615 | 16.139 | 1.00 | 118.98 | L | O |
| ATOM | 3518 | C | SER | 59 | 129.528 | -0.815 | 14.096 | 1.00 | 54.17 | L | C |
| ATOM | 3519 | O | SER | 59 | 130.015 | -0.672 | 12.970 | 1.00 | 54.17 | L | O |
| ATOM | 3520 | N | ARG | 60 | 128.861 | -1.914 | 14.449 | 1.00 | 62.94 | L | N |
| ATOM | 3521 | CA | ARG | 60 | 128.659 | -2.983 | 13.473 | 1.00 | 62.94 | L | C |
| ATOM | 3522 | CB | ARG | 60 | 128.247 | -4.291 | 14.159 | 1.00 | 67.90 | L | C |
| ATOM | 3523 | CG | ARG | 60 | 127.110 | -4.165 | 15.136 | 1.00 | 67.90 | L | C |
| ATOM | 3524 | CD | ARG | 60 | 126.572 | -5.533 | 15.506 | 1.00 | 67.90 | L | C |
| ATOM | 3525 | NE | ARG | 60 | 125.638 | -5.453 | 16.621 | 1.00 | 67.90 | L | N |
| ATOM | 3526 | CZ | ARG | 60 | 125.978 | -5.050 | 17.840 | 1.00 | 67.90 | L | C |
| ATOM | 3527 | NH1 | ARG | 60 | 127.230 | -4.696 | 18.093 | 1.00 | 67.90 | L | N |
| ATOM | 3528 | NH2 | ARG | 60 | 125.070 | -5.002 | 18.807 | 1.00 | 67.90 | L | N |
| ATOM | 3529 | C | ARG | 60 | 127.596 | -2.555 | 12.459 | 1.00 | 62.94 | L | C |
| ATOM | 3530 | O | ARG | 60 | 127.471 | -3.146 | 11.382 | 1.00 | 62.94 | L | O |
| ATOM | 3531 | N | PHE | 61 | 126.839 | -1.517 | 12.814 | 1.00 | 65.80 | L | N |
| ATOM | 3532 | CA | PHE | 61 | 125.799 | -0.979 | 11.943 | 1.00 | 65.80 | L | C |
| ATOM | 3533 | CB | PHE | 61 | 124.718 | -0.270 | 12.752 | 1.00 | 20.54 | L | C |
| ATOM | 3534 | CG | PHE | 61 | 123.650 | -1.177 | 13.278 | 1.00 | 20.54 | L | C |
| ATOM | 3535 | CD1 | PHE | 61 | 123.613 | -1.519 | 14.628 | 1.00 | 20.54 | L | C |
| ATOM | 3536 | CD2 | PHE | 61 | 122.656 | -1.662 | 12.428 | 1.00 | 20.54 | L | C |
| ATOM | 3537 | CE1 | PHE | 61 | 122.593 | -2.330 | 15.133 | 1.00 | 20.54 | L | C |
| ATOM | 3538 | CE2 | PHE | 61 | 121.627 | -2.476 | 12.914 | 1.00 | 20.54 | L | C |
| ATOM | 3539 | CZ | PHE | 61 | 121.594 | -2.809 | 14.270 | 1.00 | 20.54 | L | C |
| ATOM | 3540 | C | PHE | 61 | 126.389 | 0.019 | 10.964 | 1.00 | 65.80 | L | C |
| ATOM | 3541 | O | PHE | 61 | 127.300 | 0.773 | 11.300 | 1.00 | 65.80 | L | O |
| ATOM | 3542 | N | SER | 62 | 125.851 | 0.030 | 9.754 | 1.00 | 31.43 | L | N |
| ATOM | 3543 | CA | SER | 62 | 126.317 | 0.941 | 8.722 | 1.00 | 31.43 | L | C |
| ATOM | 3544 | CB | SER | 62 | 127.530 | 0.355 | 8.001 | 1.00 | 48.53 | L | C |
| ATOM | 3545 | OG | SER | 62 | 127.212 | -0.890 | 7.412 | 1.00 | 48.53 | L | O |
| ATOM | 3546 | C | SER | 62 | 125.211 | 1.216 | 7.714 | 1.00 | 31.43 | L | C |
| ATOM | 3547 | O | SER | 62 | 124.402 | 0.340 | 7.395 | 1.00 | 31.43 | L | O |
| ATOM | 3548 | N | GLY | 63 | 125.177 | 2.443 | 7.216 | 1.00 | 26.27 | L | N |
| ATOM | 3549 | CA | GLY | 63 | 124.168 | 2.802 | 6.244 | 1.00 | 26.27 | L | C |
| ATOM | 3550 | C | GLY | 63 | 124.870 | 3.245 | 4.988 | 1.00 | 26.27 | L | C |
| ATOM | 3551 | O | GLY | 63 | 126.032 | 3.634 | 5.044 | 1.00 | 26.27 | L | O |
| ATOM | 3552 | N | SER | 64 | 124.177 | 3.201 | 3.860 | 1.00 | 35.51 | L | N |
| ATOM | 3553 | CA | SER | 64 | 124.789 | 3.605 | 2.610 | 1.00 | 35.51 | L | C |
| ATOM | 3554 | CB | SER | 64 | 125.824 | 2.565 | 2.193 | 1.00 | 33.46 | L | C |
| ATOM | 3555 | OG | SER | 64 | 126.422 | 2.920 | 0.964 | 1.00 | 33.46 | L | O |
| ATOM | 3556 | C | SER | 64 | 123.772 | 3.783 | 1.495 | 1.00 | 35.51 | L | C |
| ATOM | 3557 | O | SER | 64 | 122.614 | 3.371 | 1.622 | 1.00 | 35.51 | L | O |
| ATOM | 3558 | N | GLY | 65 | 124.209 | 4.401 | 0.401 | 1.00 | 29.14 | L | N |
| ATOM | 3559 | CA | GLY | 65 | 123.318 | 4.594 | -0.727 | 1.00 | 29.14 | L | C |
| ATOM | 3560 | C | GLY | 65 | 123.334 | 5.963 | -1.370 | 1.00 | 29.14 | L | C |
| ATOM | 3561 | O | GLY | 65 | 124.127 | 6.837 | -1.024 | 1.00 | 29.14 | L | O |
| ATOM | 3562 | N | SER | 66 | 122.439 | 6.137 | -2.329 | 1.00 | 15.93 | L | N |
| ATOM | 3563 | CA | SER | 66 | 122.305 | 7.389 | -3.052 | 1.00 | 15.93 | L | C |
| ATOM | 3564 | CB | SER | 66 | 123.623 | 7.750 | -3.741 | 1.00 | 32.28 | L | C |
| ATOM | 3565 | OG | SER | 66 | 124.127 | 6.657 | -4.482 | 1.00 | 32.28 | L | O |
| ATOM | 3566 | C | SER | 66 | 121.171 | 7.264 | -4.076 | 1.00 | 15.93 | L | C |
| ATOM | 3567 | O | SER | 66 | 120.609 | 6.184 | -4.284 | 1.00 | 15.93 | L | O |
| ATOM | 3568 | N | GLY | 67 | 120.812 | 8.378 | -4.690 | 1.00 | 33.97 | L | N |
| ATOM | 3569 | CA | GLY | 67 | 119.751 | 8.349 | -5.673 | 1.00 | 33.97 | L | C |
| ATOM | 3570 | C | GLY | 67 | 118.469 | 7.706 | -5.194 | 1.00 | 33.97 | L | C |
| ATOM | 3571 | O | GLY | 67 | 117.757 | 8.262 | -4.361 | 1.00 | 33.97 | L | O |
| ATOM | 3572 | N | THR | 68 | 118.182 | 6.521 | -5.715 | 1.00 | 25.46 | L | N |
| ATOM | 3573 | CA | THR | 68 | 116.954 | 5.828 | -5.366 | 1.00 | 25.46 | L | C |
| ATOM | 3574 | CB | THR | 68 | 116.176 | 5.455 | -6.633 | 1.00 | 47.05 | L | C |
| ATOM | 3575 | OG1 | THR | 68 | 117.003 | 4.636 | -7.471 | 1.00 | 47.05 | L | O |
| ATOM | 3576 | CG2 | THR | 68 | 115.772 | 6.704 | -7.395 | 1.00 | 47.05 | L | C |
| ATOM | 3577 | C | THR | 68 | 117.132 | 4.559 | -4.539 | 1.00 | 25.46 | L | C |

Fig. 19: A-50

| | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 3578 | O | THR | 68 | 116.144 | 3.963 | -4.103 | 1.00 | 25.46 | L | O |
| ATOM | 3579 | N | ASP | 69 | 118.374 | 4.134 | -4.327 | 1.00 | 17.04 | L | N |
| ATOM | 3580 | CA | ASP | 69 | 118.614 | 2.921 | -3.554 | 1.00 | 17.04 | L | C |
| ATOM | 3581 | CB | ASP | 69 | 119.156 | 1.812 | -4.463 | 1.00 | 63.22 | L | C |
| ATOM | 3582 | CG | ASP | 69 | 118.129 | 1.354 | -5.490 | 1.00 | 63.22 | L | C |
| ATOM | 3583 | OD1 | ASP | 69 | 117.087 | 0.791 | -5.083 | 1.00 | 63.22 | L | O |
| ATOM | 3584 | OD2 | ASP | 69 | 118.356 | 1.565 | -6.703 | 1.00 | 63.22 | L | O |
| ATOM | 3585 | C | ASP | 69 | 119.544 | 3.146 | -2.372 | 1.00 | 17.04 | L | C |
| ATOM | 3586 | O | ASP | 69 | 120.684 | 3.567 | -2.535 | 1.00 | 17.04 | L | O |
| ATOM | 3587 | N | TYR | 70 | 119.030 | 2.866 | -1.177 | 1.00 | 19.76 | L | N |
| ATOM | 3588 | CA | TYR | 70 | 119.778 | 3.037 | 0.061 | 1.00 | 19.76 | L | C |
| ATOM | 3589 | CB | TYR | 70 | 119.130 | 4.151 | 0.895 | 1.00 | 24.73 | L | C |
| ATOM | 3590 | CG | TYR | 70 | 119.424 | 5.544 | 0.369 | 1.00 | 24.73 | L | C |
| ATOM | 3591 | CD1 | TYR | 70 | 120.547 | 6.255 | 0.809 | 1.00 | 24.73 | L | C |
| ATOM | 3592 | CE1 | TYR | 70 | 120.865 | 7.511 | 0.281 | 1.00 | 24.73 | L | C |
| ATOM | 3593 | CD2 | TYR | 70 | 118.620 | 6.129 | -0.616 | 1.00 | 24.73 | L | C |
| ATOM | 3594 | CE2 | TYR | 70 | 118.931 | 7.384 | -1.153 | 1.00 | 24.73 | L | C |
| ATOM | 3595 | CZ | TYR | 70 | 120.053 | 8.062 | -0.700 | 1.00 | 24.73 | L | C |
| ATOM | 3596 | OH | TYR | 70 | 120.371 | 9.275 | -1.247 | 1.00 | 24.73 | L | O |
| ATOM | 3597 | C | TYR | 70 | 119.812 | 1.727 | 0.840 | 1.00 | 19.76 | L | C |
| ATOM | 3598 | O | TYR | 70 | 118.997 | 0.828 | 0.599 | 1.00 | 19.76 | L | O |
| ATOM | 3599 | N | THR | 71 | 120.751 | 1.603 | 1.772 | 1.00 | 26.87 | L | N |
| ATOM | 3600 | CA | THR | 71 | 120.837 | 0.366 | 2.535 | 1.00 | 26.87 | L | C |
| ATOM | 3601 | CB | THR | 71 | 121.754 | -0.661 | 1.828 | 1.00 | 34.85 | L | C |
| ATOM | 3602 | OG1 | THR | 71 | 123.107 | -0.192 | 1.860 | 1.00 | 34.85 | L | O |
| ATOM | 3603 | CG2 | THR | 71 | 121.329 | -0.863 | 0.376 | 1.00 | 34.85 | L | C |
| ATOM | 3604 | C | THR | 71 | 121.333 | 0.483 | 3.977 | 1.00 | 26.87 | L | C |
| ATOM | 3605 | O | THR | 71 | 122.160 | 1.335 | 4.306 | 1.00 | 26.87 | L | O |
| ATOM | 3606 | N | LEU | 72 | 120.800 | -0.385 | 4.829 | 1.00 | 24.40 | L | N |
| ATOM | 3607 | CA | LEU | 72 | 121.204 | -0.467 | 6.222 | 1.00 | 24.40 | L | C |
| ATOM | 3608 | CB | LEU | 72 | 119.987 | -0.412 | 7.150 | 1.00 | 25.91 | L | C |
| ATOM | 3609 | CG | LEU | 72 | 120.183 | -0.827 | 8.614 | 1.00 | 25.91 | L | C |
| ATOM | 3610 | CD1 | LEU | 72 | 121.539 | -0.387 | 9.105 | 1.00 | 25.91 | L | C |
| ATOM | 3611 | CD2 | LEU | 72 | 119.097 | -0.207 | 9.470 | 1.00 | 25.91 | L | C |
| ATOM | 3612 | C | LEU | 72 | 121.875 | -1.837 | 6.296 | 1.00 | 24.40 | L | C |
| ATOM | 3613 | O | LEU | 72 | 121.386 | -2.803 | 5.707 | 1.00 | 24.40 | L | O |
| ATOM | 3614 | N | THR | 73 | 123.000 | -1.930 | 6.990 | 1.00 | 38.15 | L | N |
| ATOM | 3615 | CA | THR | 73 | 123.695 | -3.204 | 7.066 | 1.00 | 38.15 | L | C |
| ATOM | 3616 | CB | THR | 73 | 124.907 | -3.217 | 6.110 | 1.00 | 35.63 | L | C |
| ATOM | 3617 | OG1 | THR | 73 | 124.556 | -2.566 | 4.885 | 1.00 | 35.63 | L | O |
| ATOM | 3618 | CG2 | THR | 73 | 125.328 | -4.649 | 5.797 | 1.00 | 35.63 | L | C |
| ATOM | 3619 | C | THR | 73 | 124.189 | -3.542 | 8.467 | 1.00 | 38.15 | L | C |
| ATOM | 3620 | O | THR | 73 | 124.719 | -2.690 | 9.177 | 1.00 | 38.15 | L | O |
| ATOM | 3621 | N | ILE | 74 | 123.997 | -4.791 | 8.866 | 1.00 | 31.55 | L | N |
| ATOM | 3622 | CA | ILE | 74 | 124.467 | -5.246 | 10.158 | 1.00 | 31.55 | L | C |
| ATOM | 3623 | CB | ILE | 74 | 123.342 | -5.884 | 10.988 | 1.00 | 39.02 | L | C |
| ATOM | 3624 | CG2 | ILE | 74 | 123.734 | -5.878 | 12.461 | 1.00 | 39.02 | L | C |
| ATOM | 3625 | CG1 | ILE | 74 | 122.041 | -5.099 | 10.821 | 1.00 | 39.02 | L | C |
| ATOM | 3626 | CD1 | ILE | 74 | 120.870 | -5.663 | 11.635 | 1.00 | 39.02 | L | C |
| ATOM | 3627 | C | ILE | 74 | 125.504 | -6.313 | 9.814 | 1.00 | 31.55 | L | C |
| ATOM | 3628 | O | ILE | 74 | 125.146 | -7.434 | 9.440 | 1.00 | 31.55 | L | O |
| ATOM | 3629 | N | SER | 75 | 126.782 | -5.951 | 9.921 | 1.00 | 48.74 | L | N |
| ATOM | 3630 | CA | SER | 75 | 127.888 | -6.857 | 9.605 | 1.00 | 48.74 | L | C |
| ATOM | 3631 | CB | SER | 75 | 129.209 | -6.106 | 9.727 | 1.00 | 44.70 | L | C |
| ATOM | 3632 | OG | SER | 75 | 129.306 | -5.485 | 10.994 | 1.00 | 44.70 | L | O |
| ATOM | 3633 | C | SER | 75 | 127.940 | -8.129 | 10.456 | 1.00 | 48.74 | L | C |
| ATOM | 3634 | O | SER | 75 | 128.346 | -9.184 | 9.970 | 1.00 | 48.74 | L | O |
| ATOM | 3635 | N | SER | 76 | 127.544 | -8.021 | 11.722 | 1.00 | 53.77 | L | N |
| ATOM | 3636 | CA | SER | 76 | 127.530 | -9.165 | 12.635 | 1.00 | 53.77 | L | C |
| ATOM | 3637 | CB | SER | 76 | 128.773 | -9.166 | 13.521 | 1.00 | 79.21 | L | C |
| ATOM | 3638 | OG | SER | 76 | 128.707 | -10.224 | 14.463 | 1.00 | 79.21 | L | O |
| ATOM | 3639 | C | SER | 76 | 126.288 | -9.102 | 13.515 | 1.00 | 53.77 | L | C |
| ATOM | 3640 | O | SER | 76 | 126.306 | -8.533 | 14.604 | 1.00 | 53.77 | L | O |
| ATOM | 3641 | N | LEU | 77 | 125.211 | -9.704 | 13.036 | 1.00 | 35.38 | L | N |
| ATOM | 3642 | CA | LEU | 77 | 123.946 | -9.691 | 13.756 | 1.00 | 35.38 | L | C |
| ATOM | 3643 | CB | LEU | 77 | 122.955 | -10.639 | 13.085 | 1.00 | 37.68 | L | C |
| ATOM | 3644 | CG | LEU | 77 | 121.514 | -10.154 | 12.995 | 1.00 | 37.68 | L | C |
| ATOM | 3645 | CD1 | LEU | 77 | 120.623 | -11.329 | 12.638 | 1.00 | 37.68 | L | C |
| ATOM | 3646 | CD2 | LEU | 77 | 121.080 | -9.548 | 14.317 | 1.00 | 37.68 | L | C |
| ATOM | 3647 | C | LEU | 77 | 124.096 | -10.080 | 15.215 | 1.00 | 35.38 | L | C |
| ATOM | 3648 | O | LEU | 77 | 124.714 | -11.086 | 15.531 | 1.00 | 35.38 | L | O |
| ATOM | 3649 | N | GLN | 78 | 123.527 | -9.279 | 16.105 | 1.00 | 50.91 | L | N |
| ATOM | 3650 | CA | GLN | 78 | 123.589 | -9.577 | 17.527 | 1.00 | 50.91 | L | C |

Fig. 19: A-51

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 3651 | CB | GLN | 78 | 124.201 | -8.408 | 18.290 | 1.00 | 82.93 | L | C |
| ATOM | 3652 | CG | GLN | 78 | 125.653 | -8.159 | 17.938 | 1.00 | 82.93 | L | C |
| ATOM | 3653 | CD | GLN | 78 | 126.525 | -9.385 | 18.135 | 1.00 | 82.93 | L | C |
| ATOM | 3654 | OE1 | GLN | 78 | 126.509 | -10.007 | 19.200 | 1.00 | 82.93 | L | O |
| ATOM | 3655 | NE2 | GLN | 78 | 127.299 | -9.736 | 17.109 | 1.00 | 82.93 | L | N |
| ATOM | 3656 | C | GLN | 78 | 122.192 | -9.880 | 18.062 | 1.00 | 50.91 | L | C |
| ATOM | 3657 | O | GLN | 78 | 121.197 | -9.411 | 17.519 | 1.00 | 50.91 | L | O |
| ATOM | 3658 | N | PRO | 79 | 122.104 | -10.680 | 19.135 | 1.00 | 74.65 | L | N |
| ATOM | 3659 | CD | PRO | 79 | 123.228 | -11.171 | 19.952 | 1.00 | 43.98 | L | C |
| ATOM | 3660 | CA | PRO | 79 | 120.821 | -11.049 | 19.743 | 1.00 | 74.65 | L | C |
| ATOM | 3661 | CB | PRO | 79 | 121.243 | -11.963 | 20.887 | 1.00 | 43.98 | L | C |
| ATOM | 3662 | CG | PRO | 79 | 122.577 | -11.373 | 21.284 | 1.00 | 43.98 | L | C |
| ATOM | 3663 | C | PRO | 79 | 120.033 | -9.830 | 20.224 | 1.00 | 74.65 | L | C |
| ATOM | 3664 | O | PRO | 79 | 118.855 | -9.922 | 20.577 | 1.00 | 74.65 | L | O |
| ATOM | 3665 | N | GLU | 80 | 120.697 | -8.685 | 20.221 | 1.00 | 42.25 | L | N |
| ATOM | 3666 | CA | GLU | 80 | 120.080 | -7.451 | 20.659 | 1.00 | 42.25 | L | C |
| ATOM | 3667 | CB | GLU | 80 | 121.085 | -6.697 | 21.527 | 1.00 | 40.93 | L | C |
| ATOM | 3668 | CG | GLU | 80 | 122.485 | -6.700 | 20.958 | 1.00 | 40.93 | L | C |
| ATOM | 3669 | CD | GLU | 80 | 123.424 | -5.786 | 21.726 | 1.00 | 40.93 | L | C |
| ATOM | 3670 | OE1 | GLU | 80 | 123.013 | -4.648 | 22.033 | 1.00 | 40.93 | L | O |
| ATOM | 3671 | OE2 | GLU | 80 | 124.572 | -6.197 | 22.009 | 1.00 | 40.93 | L | O |
| ATOM | 3672 | C | GLU | 80 | 119.602 | -6.575 | 19.489 | 1.00 | 42.25 | L | C |
| ATOM | 3673 | O | GLU | 80 | 118.723 | -5.726 | 19.656 | 1.00 | 42.25 | L | O |
| ATOM | 3674 | N | ASP | 81 | 120.189 | -6.787 | 18.312 | 1.00 | 42.48 | L | N |
| ATOM | 3675 | CA | ASP | 81 | 119.835 | -6.037 | 17.108 | 1.00 | 42.48 | L | C |
| ATOM | 3676 | CB | ASP | 81 | 120.867 | -6.254 | 16.005 | 1.00 | 43.12 | L | C |
| ATOM | 3677 | CG | ASP | 81 | 122.262 | -5.914 | 16.441 | 1.00 | 43.12 | L | C |
| ATOM | 3678 | OD1 | ASP | 81 | 122.422 | -5.003 | 17.281 | 1.00 | 43.12 | L | O |
| ATOM | 3679 | OD2 | ASP | 81 | 123.205 | -6.549 | 15.924 | 1.00 | 43.12 | L | O |
| ATOM | 3680 | C | ASP | 81 | 118.495 | -6.488 | 16.564 | 1.00 | 42.48 | L | C |
| ATOM | 3681 | O | ASP | 81 | 118.086 | -6.063 | 15.488 | 1.00 | 42.48 | L | O |
| ATOM | 3682 | N | PHE | 82 | 117.810 | -7.351 | 17.299 | 1.00 | 48.53 | L | N |
| ATOM | 3683 | CA | PHE | 82 | 116.544 | -7.856 | 16.822 | 1.00 | 48.53 | L | C |
| ATOM | 3684 | CB | PHE | 82 | 116.337 | -9.265 | 17.368 | 1.00 | 189.91 | L | C |
| ATOM | 3685 | CG | PHE | 82 | 117.320 | -10.260 | 16.810 | 1.00 | 189.91 | L | C |
| ATOM | 3686 | CD1 | PHE | 82 | 117.227 | -10.676 | 15.485 | 1.00 | 189.91 | L | C |
| ATOM | 3687 | CD2 | PHE | 82 | 118.369 | -10.741 | 17.587 | 1.00 | 189.91 | L | C |
| ATOM | 3688 | CE1 | PHE | 82 | 118.164 | -11.554 | 14.940 | 1.00 | 189.91 | L | C |
| ATOM | 3689 | CE2 | PHE | 82 | 119.311 | -11.622 | 17.048 | 1.00 | 189.91 | L | C |
| ATOM | 3690 | CZ | PHE | 82 | 119.207 | -12.027 | 15.725 | 1.00 | 189.91 | L | C |
| ATOM | 3691 | C | PHE | 82 | 115.359 | -6.953 | 17.094 | 1.00 | 48.53 | L | C |
| ATOM | 3692 | O | PHE | 82 | 114.857 | -6.863 | 18.216 | 1.00 | 48.53 | L | O |
| ATOM | 3693 | N | ALA | 83 | 114.939 | -6.271 | 16.032 | 1.00 | 31.52 | L | N |
| ATOM | 3694 | CA | ALA | 83 | 113.813 | -5.350 | 16.052 | 1.00 | 31.52 | L | C |
| ATOM | 3695 | CB | ALA | 83 | 114.217 | -4.051 | 16.723 | 1.00 | 63.37 | L | C |
| ATOM | 3696 | C | ALA | 83 | 113.398 | -5.090 | 14.605 | 1.00 | 31.52 | L | C |
| ATOM | 3697 | O | ALA | 83 | 113.816 | -5.808 | 13.693 | 1.00 | 31.52 | L | O |
| ATOM | 3698 | N | THR | 84 | 112.565 | -4.075 | 14.395 | 1.00 | 28.09 | L | N |
| ATOM | 3699 | CA | THR | 84 | 112.124 | -3.733 | 13.045 | 1.00 | 28.09 | L | C |
| ATOM | 3700 | CB | THR | 84 | 110.572 | -3.799 | 12.928 | 1.00 | 15.50 | L | C |
| ATOM | 3701 | OG1 | THR | 84 | 110.127 | -3.002 | 11.822 | 1.00 | 15.50 | L | O |
| ATOM | 3702 | CG2 | THR | 84 | 109.922 | -3.332 | 14.207 | 1.00 | 15.50 | L | C |
| ATOM | 3703 | C | THR | 84 | 112.664 | -2.346 | 12.659 | 1.00 | 28.09 | L | C |
| ATOM | 3704 | O | THR | 84 | 112.505 | -1.373 | 13.400 | 1.00 | 28.09 | L | O |
| ATOM | 3705 | N | TYR | 85 | 113.316 | -2.282 | 11.496 | 1.00 | 21.31 | L | N |
| ATOM | 3706 | CA | TYR | 85 | 113.935 | -1.055 | 11.000 | 1.00 | 21.31 | L | C |
| ATOM | 3707 | CB | TYR | 85 | 115.367 | -1.338 | 10.517 | 1.00 | 19.63 | L | C |
| ATOM | 3708 | CG | TYR | 85 | 116.240 | -1.976 | 11.566 | 1.00 | 19.63 | L | C |
| ATOM | 3709 | CD1 | TYR | 85 | 115.988 | -3.279 | 12.021 | 1.00 | 19.63 | L | C |
| ATOM | 3710 | CE1 | TYR | 85 | 116.718 | -3.834 | 13.061 | 1.00 | 19.63 | L | C |
| ATOM | 3711 | CD2 | TYR | 85 | 117.255 | -1.259 | 12.174 | 1.00 | 19.63 | L | C |
| ATOM | 3712 | CE2 | TYR | 85 | 117.990 | -1.807 | 13.217 | 1.00 | 19.63 | L | C |
| ATOM | 3713 | CZ | TYR | 85 | 117.711 | -3.087 | 13.655 | 1.00 | 19.63 | L | C |
| ATOM | 3714 | OH | TYR | 85 | 118.405 | -3.592 | 14.722 | 1.00 | 19.63 | L | O |
| ATOM | 3715 | C | TYR | 85 | 113.173 | -0.365 | 9.882 | 1.00 | 21.31 | L | C |
| ATOM | 3716 | O | TYR | 85 | 112.768 | -0.996 | 8.900 | 1.00 | 21.31 | L | O |
| ATOM | 3717 | N | TYR | 86 | 113.015 | 0.948 | 10.046 | 1.00 | 18.01 | L | N |
| ATOM | 3718 | CA | TYR | 86 | 112.321 | 1.806 | 9.090 | 1.00 | 18.01 | L | C |
| ATOM | 3719 | CB | TYR | 86 | 111.242 | 2.632 | 9.790 | 1.00 | 24.73 | L | C |
| ATOM | 3720 | CG | TYR | 86 | 110.130 | 1.846 | 10.421 | 1.00 | 24.73 | L | C |
| ATOM | 3721 | CD1 | TYR | 86 | 109.020 | 1.459 | 9.679 | 1.00 | 24.73 | L | C |
| ATOM | 3722 | CE1 | TYR | 86 | 107.971 | 0.756 | 10.278 | 1.00 | 24.73 | L | C |
| ATOM | 3723 | CD2 | TYR | 86 | 110.177 | 1.508 | 11.773 | 1.00 | 24.73 | L | C |

Fig. 19: A-52

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 3724 | CE2 | TYR | 86 | 109.140 | 0.804 | 12.378 | 1.00 | 24.73 | L | C |
| ATOM | 3725 | CZ | TYR | 86 | 108.042 | 0.438 | 11.628 | 1.00 | 24.73 | L | C |
| ATOM | 3726 | OH | TYR | 86 | 107.002 | -0.204 | 12.238 | 1.00 | 24.73 | L | O |
| ATOM | 3727 | C | TYR | 86 | 113.280 | 2.798 | 8.465 | 1.00 | 18.01 | L | C |
| ATOM | 3728 | O | TYR | 86 | 114.110 | 3.378 | 9.158 | 1.00 | 18.01 | L | O |
| ATOM | 3729 | N | CYS | 87 | 113.170 | 2.996 | 7.158 | 1.00 | 20.53 | L | N |
| ATOM | 3730 | CA | CYS | 87 | 113.989 | 3.999 | 6.494 | 1.00 | 20.53 | L | C |
| ATOM | 3731 | C | CYS | 87 | 113.021 | 5.156 | 6.335 | 1.00 | 20.53 | L | C |
| ATOM | 3732 | O | CYS | 87 | 111.806 | 4.954 | 6.351 | 1.00 | 20.53 | L | O |
| ATOM | 3733 | CB | CYS | 87 | 114.509 | 3.527 | 5.133 | 1.00 | 17.33 | L | C |
| ATOM | 3734 | SG | CYS | 87 | 113.306 | 2.900 | 3.921 | 1.00 | 17.33 | L | S |
| ATOM | 3735 | N | GLN | 88 | 113.545 | 6.363 | 6.212 | 1.00 | 10.63 | L | N |
| ATOM | 3736 | CA | GLN | 88 | 112.696 | 7.534 | 6.083 | 1.00 | 10.63 | L | C |
| ATOM | 3737 | CB | GLN | 88 | 112.393 | 8.083 | 7.482 | 1.00 | 18.09 | L | C |
| ATOM | 3738 | CG | GLN | 88 | 111.509 | 9.303 | 7.525 | 1.00 | 18.09 | L | C |
| ATOM | 3739 | CD | GLN | 88 | 112.256 | 10.547 | 7.971 | 1.00 | 18.09 | L | C |
| ATOM | 3740 | OE1 | GLN | 88 | 112.946 | 10.539 | 8.987 | 1.00 | 18.09 | L | O |
| ATOM | 3741 | NE2 | GLN | 88 | 112.106 | 11.627 | 7.219 | 1.00 | 18.09 | L | N |
| ATOM | 3742 | C | GLN | 88 | 113.390 | 8.583 | 5.219 | 1.00 | 10.63 | L | C |
| ATOM | 3743 | O | GLN | 88 | 114.626 | 8.680 | 5.198 | 1.00 | 10.63 | L | O |
| ATOM | 3744 | N | GLN | 89 | 112.600 | 9.357 | 4.483 | 1.00 | 11.94 | L | N |
| ATOM | 3745 | CA | GLN | 89 | 113.171 | 10.386 | 3.625 | 1.00 | 11.94 | L | C |
| ATOM | 3746 | CB | GLN | 89 | 112.877 | 10.073 | 2.152 | 1.00 | 25.01 | L | C |
| ATOM | 3747 | CG | GLN | 89 | 111.407 | 10.008 | 1.776 | 1.00 | 25.01 | L | C |
| ATOM | 3748 | CD | GLN | 89 | 110.786 | 11.377 | 1.579 | 1.00 | 25.01 | L | C |
| ATOM | 3749 | OE1 | GLN | 89 | 111.373 | 12.247 | 0.935 | 1.00 | 25.01 | L | O |
| ATOM | 3750 | NE2 | GLN | 89 | 109.591 | 11.571 | 2.119 | 1.00 | 25.01 | L | N |
| ATOM | 3751 | C | GLN | 89 | 112.606 | 11.732 | 4.023 | 1.00 | 11.94 | L | C |
| ATOM | 3752 | O | GLN | 89 | 111.498 | 11.802 | 4.552 | 1.00 | 11.94 | L | O |
| ATOM | 3753 | N | TRP | 90 | 113.375 | 12.794 | 3.792 | 1.00 | 19.62 | L | N |
| ATOM | 3754 | CA | TRP | 90 | 112.948 | 14.144 | 4.145 | 1.00 | 19.62 | L | C |
| ATOM | 3755 | CB | TRP | 90 | 113.773 | 14.667 | 5.336 | 1.00 | 17.27 | L | C |
| ATOM | 3756 | CG | TRP | 90 | 115.220 | 15.018 | 5.023 | 1.00 | 17.27 | L | C |
| ATOM | 3757 | CD2 | TRP | 90 | 116.174 | 15.611 | 5.918 | 1.00 | 17.27 | L | C |
| ATOM | 3758 | CE2 | TRP | 90 | 117.373 | 15.797 | 5.189 | 1.00 | 17.27 | L | C |
| ATOM | 3759 | CE3 | TRP | 90 | 116.132 | 16.005 | 7.267 | 1.00 | 17.27 | L | C |
| ATOM | 3760 | CD1 | TRP | 90 | 115.869 | 14.867 | 3.823 | 1.00 | 17.27 | L | C |
| ATOM | 3761 | NE1 | TRP | 90 | 117.156 | 15.334 | 3.918 | 1.00 | 17.27 | L | N |
| ATOM | 3762 | CZ2 | TRP | 90 | 118.522 | 16.363 | 5.759 | 1.00 | 17.27 | L | C |
| ATOM | 3763 | CZ3 | TRP | 90 | 117.284 | 16.570 | 7.839 | 1.00 | 17.27 | L | C |
| ATOM | 3764 | CH2 | TRP | 90 | 118.462 | 16.741 | 7.080 | 1.00 | 17.27 | L | C |
| ATOM | 3765 | C | TRP | 90 | 113.074 | 15.093 | 2.947 | 1.00 | 19.62 | L | C |
| ATOM | 3766 | O | TRP | 90 | 112.783 | 16.289 | 3.048 | 1.00 | 19.62 | L | O |
| ATOM | 3767 | N | SER | 91 | 113.494 | 14.552 | 1.807 | 1.00 | 12.71 | L | N |
| ATOM | 3768 | CA | SER | 91 | 113.662 | 15.359 | 0.600 | 1.00 | 12.71 | L | C |
| ATOM | 3769 | CB | SER | 91 | 114.504 | 14.587 | -0.414 | 1.00 | 23.55 | L | C |
| ATOM | 3770 | OG | SER | 91 | 115.762 | 14.248 | 0.137 | 1.00 | 23.55 | L | O |
| ATOM | 3771 | C | SER | 91 | 112.344 | 15.800 | -0.054 | 1.00 | 12.71 | L | C |
| ATOM | 3772 | O | SER | 91 | 112.284 | 16.860 | -0.680 | 1.00 | 12.71 | L | O |
| ATOM | 3773 | N | GLY | 92 | 111.297 | 14.986 | 0.096 | 1.00 | 23.24 | L | N |
| ATOM | 3774 | CA | GLY | 92 | 110.008 | 15.310 | -0.493 | 1.00 | 23.24 | L | C |
| ATOM | 3775 | C | GLY | 92 | 108.867 | 15.347 | 0.509 | 1.00 | 23.24 | L | C |
| ATOM | 3776 | O | GLY | 92 | 108.931 | 14.718 | 1.567 | 1.00 | 23.24 | L | O |
| ATOM | 3777 | N | ASN | 93 | 107.811 | 16.078 | 0.169 | 1.00 | 31.94 | L | N |
| ATOM | 3778 | CA | ASN | 93 | 106.663 | 16.206 | 1.048 | 1.00 | 31.94 | L | C |
| ATOM | 3779 | CB | ASN | 93 | 106.307 | 17.670 | 1.203 | 1.00 | 23.71 | L | C |
| ATOM | 3780 | CG | ASN | 93 | 107.400 | 18.448 | 1.896 | 1.00 | 23.71 | L | C |
| ATOM | 3781 | OD1 | ASN | 93 | 107.790 | 19.525 | 1.445 | 1.00 | 23.71 | L | O |
| ATOM | 3782 | ND2 | ASN | 93 | 107.905 | 17.905 | 3.006 | 1.00 | 23.71 | L | N |
| ATOM | 3783 | C | ASN | 93 | 105.478 | 15.454 | 0.507 | 1.00 | 31.94 | L | C |
| ATOM | 3784 | O | ASN | 93 | 105.227 | 15.478 | -0.692 | 1.00 | 31.94 | L | O |
| ATOM | 3785 | N | PRO | 94 | 104.724 | 14.779 | 1.386 | 1.00 | 29.10 | L | N |
| ATOM | 3786 | CD | PRO | 94 | 103.575 | 13.939 | 1.009 | 1.00 | 1.87 | L | C |
| ATOM | 3787 | CA | PRO | 94 | 104.950 | 14.713 | 2.830 | 1.00 | 29.10 | L | C |
| ATOM | 3788 | CB | PRO | 94 | 103.651 | 14.113 | 3.340 | 1.00 | 1.87 | L | C |
| ATOM | 3789 | CG | PRO | 94 | 103.336 | 13.137 | 2.269 | 1.00 | 1.87 | L | C |
| ATOM | 3790 | C | PRO | 94 | 106.131 | 13.823 | 3.167 | 1.00 | 29.10 | L | C |
| ATOM | 3791 | O | PRO | 94 | 106.516 | 12.987 | 2.361 | 1.00 | 29.10 | L | O |
| ATOM | 3792 | N | TRP | 95 | 106.711 | 14.011 | 4.349 | 1.00 | 16.41 | L | N |
| ATOM | 3793 | CA | TRP | 95 | 107.810 | 13.155 | 4.772 | 1.00 | 16.41 | L | C |
| ATOM | 3794 | CB | TRP | 95 | 108.425 | 13.629 | 6.094 | 1.00 | 13.37 | L | C |
| ATOM | 3795 | CG | TRP | 95 | 109.201 | 14.906 | 5.979 | 1.00 | 13.37 | L | C |
| ATOM | 3796 | CD2 | TRP | 95 | 109.284 | 15.950 | 6.954 | 1.00 | 13.37 | L | C |

Fig. 19: A-53

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 3797 | CE2 | TRP | 95 | 110.104 | 16.960 | 6.412 | 1.00 | 13.37 | L | C |
| ATOM | 3798 | CE3 | TRP | 95 | 108.743 | 16.132 | 8.229 | 1.00 | 13.37 | L | C |
| ATOM | 3799 | CD1 | TRP | 95 | 109.963 | 15.312 | 4.917 | 1.00 | 13.37 | L | C |
| ATOM | 3800 | NE1 | TRP | 95 | 110.504 | 16.543 | 5.168 | 1.00 | 13.37 | L | N |
| ATOM | 3801 | CZ2 | TRP | 95 | 110.394 | 18.144 | 7.107 | 1.00 | 13.37 | L | C |
| ATOM | 3802 | CZ3 | TRP | 95 | 109.030 | 17.305 | 8.919 | 1.00 | 13.37 | L | C |
| ATOM | 3803 | CH2 | TRP | 95 | 109.845 | 18.297 | 8.358 | 1.00 | 13.37 | L | C |
| ATOM | 3804 | C | TRP | 95 | 107.226 | 11.751 | 4.942 | 1.00 | 16.41 | L | C |
| ATOM | 3805 | O | TRP | 95 | 106.136 | 11.575 | 5.484 | 1.00 | 16.41 | L | O |
| ATOM | 3806 | N | THR | 96 | 107.956 | 10.748 | 4.481 | 1.00 | 6.71 | L | N |
| ATOM | 3807 | CA | THR | 96 | 107.465 | 9.388 | 4.563 | 1.00 | 6.71 | L | C |
| ATOM | 3808 | CB | THR | 96 | 106.963 | 8.932 | 3.172 | 1.00 | 11.59 | L | C |
| ATOM | 3809 | OG1 | THR | 96 | 108.045 | 8.991 | 2.235 | 1.00 | 11.59 | L | O |
| ATOM | 3810 | CG2 | THR | 96 | 105.859 | 9.852 | 2.674 | 1.00 | 11.59 | L | C |
| ATOM | 3811 | C | THR | 96 | 108.489 | 8.369 | 5.087 | 1.00 | 6.71 | L | C |
| ATOM | 3812 | O | THR | 96 | 109.703 | 8.621 | 5.121 | 1.00 | 6.71 | L | O |
| ATOM | 3813 | N | PHE | 97 | 107.966 | 7.222 | 5.513 | 1.00 | 24.36 | L | N |
| ATOM | 3814 | CA | PHE | 97 | 108.777 | 6.119 | 6.013 | 1.00 | 24.36 | L | C |
| ATOM | 3815 | CB | PHE | 97 | 108.327 | 5.689 | 7.418 | 1.00 | 11.10 | L | C |
| ATOM | 3816 | CG | PHE | 97 | 108.422 | 6.762 | 8.461 | 1.00 | 11.10 | L | C |
| ATOM | 3817 | CD1 | PHE | 97 | 107.541 | 7.831 | 8.460 | 1.00 | 11.10 | L | C |
| ATOM | 3818 | CD2 | PHE | 97 | 109.391 | 6.685 | 9.470 | 1.00 | 11.10 | L | C |
| ATOM | 3819 | CE1 | PHE | 97 | 107.612 | 8.821 | 9.453 | 1.00 | 11.10 | L | C |
| ATOM | 3820 | CE2 | PHE | 97 | 109.475 | 7.665 | 10.468 | 1.00 | 11.10 | L | C |
| ATOM | 3821 | CZ | PHE | 97 | 108.577 | 8.738 | 10.456 | 1.00 | 11.10 | L | C |
| ATOM | 3822 | C | PHE | 97 | 108.532 | 4.950 | 5.062 | 1.00 | 24.36 | L | C |
| ATOM | 3823 | O | PHE | 97 | 107.613 | 4.990 | 4.241 | 1.00 | 24.36 | L | O |
| ATOM | 3824 | N | GLY | 98 | 109.362 | 3.919 | 5.168 | 1.00 | 21.54 | L | N |
| ATOM | 3825 | CA | GLY | 98 | 109.183 | 2.727 | 4.350 | 1.00 | 21.54 | L | C |
| ATOM | 3826 | C | GLY | 98 | 108.266 | 1.849 | 5.184 | 1.00 | 21.54 | L | C |
| ATOM | 3827 | O | GLY | 98 | 107.977 | 2.196 | 6.339 | 1.00 | 21.54 | L | O |
| ATOM | 3828 | N | GLN | 99 | 107.796 | 0.728 | 4.645 | 1.00 | 11.59 | L | N |
| ATOM | 3829 | CA | GLN | 99 | 106.894 | -0.114 | 5.442 | 1.00 | 11.59 | L | C |
| ATOM | 3830 | CB | GLN | 99 | 106.211 | -1.197 | 4.593 | 1.00 | 37.88 | L | C |
| ATOM | 3831 | CG | GLN | 99 | 106.810 | -1.403 | 3.238 | 1.00 | 37.88 | L | C |
| ATOM | 3832 | CD | GLN | 99 | 108.266 | -1.748 | 3.319 | 1.00 | 37.88 | L | C |
| ATOM | 3833 | OE1 | GLN | 99 | 108.638 | -2.821 | 3.796 | 1.00 | 37.88 | L | O |
| ATOM | 3834 | NE2 | GLN | 99 | 109.110 | -0.832 | 2.866 | 1.00 | 37.88 | L | N |
| ATOM | 3835 | C | GLN | 99 | 107.586 | -0.758 | 6.634 | 1.00 | 11.59 | L | C |
| ATOM | 3836 | O | GLN | 99 | 106.943 | -1.317 | 7.508 | 1.00 | 11.59 | L | O |
| ATOM | 3837 | N | GLY | 100 | 108.902 | -0.640 | 6.684 | 1.00 | 24.72 | L | N |
| ATOM | 3838 | CA | GLY | 100 | 109.633 | -1.225 | 7.785 | 1.00 | 24.72 | L | C |
| ATOM | 3839 | C | GLY | 100 | 110.055 | -2.630 | 7.425 | 1.00 | 24.72 | L | C |
| ATOM | 3840 | O | GLY | 100 | 109.402 | -3.279 | 6.606 | 1.00 | 24.72 | L | O |
| ATOM | 3841 | N | THR | 101 | 111.157 | -3.084 | 8.017 | 1.00 | 23.77 | L | N |
| ATOM | 3842 | CA | THR | 101 | 111.685 | -4.424 | 7.780 | 1.00 | 23.77 | L | C |
| ATOM | 3843 | CB | THR | 101 | 113.019 | -4.382 | 7.040 | 1.00 | 10.18 | L | C |
| ATOM | 3844 | OG1 | THR | 101 | 112.790 | -4.076 | 5.659 | 1.00 | 10.18 | L | O |
| ATOM | 3845 | CG2 | THR | 101 | 113.735 | -5.716 | 7.173 | 1.00 | 10.18 | L | C |
| ATOM | 3846 | C | THR | 101 | 111.908 | -5.076 | 9.129 | 1.00 | 23.77 | L | C |
| ATOM | 3847 | O | THR | 101 | 112.689 | -4.582 | 9.942 | 1.00 | 23.77 | L | O |
| ATOM | 3848 | N | LYS | 102 | 111.223 | -6.188 | 9.365 | 1.00 | 19.34 | L | N |
| ATOM | 3849 | CA | LYS | 102 | 111.347 | -6.858 | 10.641 | 1.00 | 19.34 | L | C |
| ATOM | 3850 | CB | LYS | 102 | 110.009 | -7.496 | 11.027 | 1.00 | 36.70 | L | C |
| ATOM | 3851 | CG | LYS | 102 | 109.872 | -7.774 | 12.521 | 1.00 | 36.70 | L | C |
| ATOM | 3852 | CD | LYS | 102 | 108.464 | -8.244 | 12.876 | 1.00 | 36.70 | L | C |
| ATOM | 3853 | CE | LYS | 102 | 108.313 | -8.467 | 14.372 | 1.00 | 36.70 | L | C |
| ATOM | 3854 | NZ | LYS | 102 | 108.632 | -7.218 | 15.120 | 1.00 | 36.70 | L | N |
| ATOM | 3855 | C | LYS | 102 | 112.449 | -7.907 | 10.608 | 1.00 | 19.34 | L | C |
| ATOM | 3856 | O | LYS | 102 | 112.530 | -8.703 | 9.661 | 1.00 | 19.34 | L | O |
| ATOM | 3857 | N | VAL | 103 | 113.304 | -7.894 | 11.634 | 1.00 | 20.01 | L | N |
| ATOM | 3858 | CA | VAL | 103 | 114.378 | -8.868 | 11.714 | 1.00 | 20.01 | L | C |
| ATOM | 3859 | CB | VAL | 103 | 115.793 | -8.188 | 11.567 | 1.00 | 24.69 | L | C |
| ATOM | 3860 | CG1 | VAL | 103 | 115.696 | -6.991 | 10.636 | 1.00 | 24.69 | L | C |
| ATOM | 3861 | CG2 | VAL | 103 | 116.361 | -7.780 | 12.908 | 1.00 | 24.69 | L | C |
| ATOM | 3862 | C | VAL | 103 | 114.280 | -9.654 | 13.031 | 1.00 | 20.01 | L | C |
| ATOM | 3863 | O | VAL | 103 | 114.380 | -9.075 | 14.117 | 1.00 | 20.01 | L | O |
| ATOM | 3864 | N | GLU | 104 | 114.047 | -10.969 | 12.927 | 1.00 | 25.78 | L | N |
| ATOM | 3865 | CA | GLU | 104 | 113.948 | -11.831 | 14.106 | 1.00 | 25.78 | L | C |
| ATOM | 3866 | CB | GLU | 104 | 112.662 | -12.666 | 14.098 | 1.00 | 117.28 | L | C |
| ATOM | 3867 | CG | GLU | 104 | 112.589 | -13.728 | 13.022 | 1.00 | 117.28 | L | C |
| ATOM | 3868 | CD | GLU | 104 | 112.095 | -13.176 | 11.705 | 1.00 | 117.28 | L | C |
| ATOM | 3869 | OE1 | GLU | 104 | 112.047 | -13.942 | 10.717 | 1.00 | 117.28 | L | O |

Fig. 19: A-54

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 3870 | OE2 | GLU | 104 | 111.747 | -11.975 | 11.660 | 1.00 | 117.28 | L | O |
| ATOM | 3871 | C | GLU | 104 | 115.148 | -12.759 | 14.179 | 1.00 | 25.78 | L | C |
| ATOM | 3872 | O | GLU | 104 | 115.852 | -12.955 | 13.185 | 1.00 | 25.78 | L | O |
| ATOM | 3873 | N | ILE | 105 | 115.368 | -13.324 | 15.365 | 1.00 | 16.82 | L | N |
| ATOM | 3874 | CA | ILE | 105 | 116.489 | -14.228 | 15.621 | 1.00 | 16.82 | L | C |
| ATOM | 3875 | CB | ILE | 105 | 116.771 | -14.386 | 17.124 | 1.00 | 41.57 | L | C |
| ATOM | 3876 | CG2 | ILE | 105 | 118.226 | -14.701 | 17.335 | 1.00 | 41.57 | L | C |
| ATOM | 3877 | CG1 | ILE | 105 | 116.372 | -13.111 | 17.873 | 1.00 | 41.57 | L | C |
| ATOM | 3878 | CD1 | ILE | 105 | 116.594 | -13.151 | 19.385 | 1.00 | 41.57 | L | C |
| ATOM | 3879 | C | ILE | 105 | 116.204 | -15.611 | 15.102 | 1.00 | 16.82 | L | C |
| ATOM | 3880 | O | ILE | 105 | 115.251 | -16.250 | 15.543 | 1.00 | 16.82 | L | O |
| ATOM | 3881 | N | LYS | 106 | 117.008 | -16.076 | 14.153 | 1.00 | 39.65 | L | N |
| ATOM | 3882 | CA | LYS | 106 | 116.807 | -17.422 | 13.653 | 1.00 | 39.65 | L | C |
| ATOM | 3883 | CB | LYS | 106 | 117.310 | -17.587 | 12.217 | 1.00 | 48.57 | L | C |
| ATOM | 3884 | CG | LYS | 106 | 116.947 | -18.952 | 11.631 | 1.00 | 48.57 | L | C |
| ATOM | 3885 | CD | LYS | 106 | 117.401 | -19.148 | 10.179 | 1.00 | 48.57 | L | C |
| ATOM | 3886 | CE | LYS | 106 | 117.087 | -20.579 | 9.702 | 1.00 | 48.57 | L | C |
| ATOM | 3887 | NZ | LYS | 106 | 117.672 | -20.948 | 8.369 | 1.00 | 48.57 | L | N |
| ATOM | 3888 | C | LYS | 106 | 117.598 | -18.310 | 14.600 | 1.00 | 39.65 | L | C |
| ATOM | 3889 | O | LYS | 106 | 118.804 | -18.122 | 14.782 | 1.00 | 38.70 | L | O |
| ATOM | 3890 | N | ARG | 107 | 116.894 | -19.242 | 15.235 | 1.00 | 14.86 | L | N |
| ATOM | 3891 | CA | ARG | 107 | 117.492 | -20.178 | 16.174 | 1.00 | 14.86 | L | C |
| ATOM | 3892 | CB | ARG | 107 | 117.158 | -19.771 | 17.605 | 1.00 | 20.96 | L | C |
| ATOM | 3893 | CG | ARG | 107 | 115.687 | -19.532 | 17.832 | 1.00 | 20.96 | L | C |
| ATOM | 3894 | CD | ARG | 107 | 115.296 | -19.930 | 19.239 | 1.00 | 20.96 | L | C |
| ATOM | 3895 | NE | ARG | 107 | 115.615 | -21.335 | 19.502 | 1.00 | 20.96 | L | N |
| ATOM | 3896 | CZ | ARG | 107 | 115.513 | -21.910 | 20.692 | 1.00 | 20.96 | L | C |
| ATOM | 3897 | NH1 | ARG | 107 | 115.096 | -21.206 | 21.732 | 1.00 | 20.96 | L | N |
| ATOM | 3898 | NH2 | ARG | 107 | 115.843 | -23.182 | 20.840 | 1.00 | 20.96 | L | N |
| ATOM | 3899 | C | ARG | 107 | 116.986 | -21.595 | 15.899 | 1.00 | 14.86 | L | C |
| ATOM | 3900 | O | ARG | 107 | 116.062 | -21.796 | 15.107 | 1.00 | 14.86 | L | O |
| ATOM | 3901 | N | THR | 108 | 117.606 | -22.575 | 16.545 | 1.00 | 15.74 | L | N |
| ATOM | 3902 | CA | THR | 108 | 117.220 | -23.963 | 16.354 | 1.00 | 15.74 | L | C |
| ATOM | 3903 | CB | THR | 108 | 118.025 | -24.921 | 17.260 | 1.00 | 26.88 | L | C |
| ATOM | 3904 | OG1 | THR | 108 | 118.232 | -24.320 | 18.548 | 1.00 | 26.88 | L | O |
| ATOM | 3905 | CG2 | THR | 108 | 119.347 | -25.257 | 16.618 | 1.00 | 26.88 | L | C |
| ATOM | 3906 | C | THR | 108 | 115.756 | -24.161 | 16.653 | 1.00 | 15.74 | L | C |
| ATOM | 3907 | O | THR | 108 | 115.179 | -23.450 | 17.481 | 1.00 | 15.74 | L | O |
| ATOM | 3908 | N | VAL | 109 | 115.170 | -25.134 | 15.963 | 1.00 | 14.98 | L | N |
| ATOM | 3909 | CA | VAL | 109 | 113.775 | -25.469 | 16.136 | 1.00 | 12.60 | L | C |
| ATOM | 3910 | CB | VAL | 109 | 113.368 | -26.593 | 15.189 | 1.00 | 15.46 | L | C |
| ATOM | 3911 | CG1 | VAL | 109 | 111.987 | -27.105 | 15.527 | 1.00 | 14.41 | L | C |
| ATOM | 3912 | CG2 | VAL | 109 | 113.383 | -26.074 | 13.789 | 1.00 | 13.59 | L | C |
| ATOM | 3913 | C | VAL | 109 | 113.517 | -25.909 | 17.565 | 1.00 | 13.54 | L | C |
| ATOM | 3914 | O | VAL | 109 | 114.393 | -26.477 | 18.236 | 1.00 | 21.28 | L | O |
| ATOM | 3915 | N | ALA | 110 | 112.313 | -25.637 | 18.036 | 1.00 | 11.81 | L | N |
| ATOM | 3916 | CA | ALA | 110 | 111.953 | -26.001 | 19.383 | 1.00 | 12.99 | L | C |
| ATOM | 3917 | CB | ALA | 110 | 112.312 | -24.878 | 20.330 | 1.00 | 8.30 | L | C |
| ATOM | 3918 | C | ALA | 110 | 110.463 | -26.281 | 19.426 | 1.00 | 13.63 | L | C |
| ATOM | 3919 | O | ALA | 110 | 109.654 | -25.390 | 19.158 | 1.00 | 15.92 | L | O |
| ATOM | 3920 | N | ALA | 111 | 110.112 | -27.525 | 19.758 | 1.00 | 25.70 | L | N |
| ATOM | 3921 | CA | ALA | 111 | 108.715 | -27.951 | 19.838 | 1.00 | 26.75 | L | C |
| ATOM | 3922 | CB | ALA | 111 | 108.641 | -29.446 | 20.087 | 1.00 | 23.32 | L | C |
| ATOM | 3923 | C | ALA | 111 | 107.981 | -27.198 | 20.936 | 1.00 | 25.59 | L | C |
| ATOM | 3924 | O | ALA | 111 | 108.525 | -26.926 | 22.008 | 1.00 | 29.44 | L | O |
| ATOM | 3925 | N | PRO | 112 | 106.720 | -26.857 | 20.686 | 1.00 | 20.76 | L | N |
| ATOM | 3926 | CD | PRO | 112 | 105.901 | -27.063 | 19.477 | 1.00 | 26.01 | L | C |
| ATOM | 3927 | CA | PRO | 112 | 105.975 | -26.125 | 21.707 | 1.00 | 26.81 | L | C |
| ATOM | 3928 | CB | PRO | 112 | 104.938 | -25.381 | 20.882 | 1.00 | 26.37 | L | C |
| ATOM | 3929 | CG | PRO | 112 | 104.550 | -26.457 | 19.876 | 1.00 | 24.71 | L | C |
| ATOM | 3930 | C | PRO | 112 | 105.322 | -27.058 | 22.703 | 1.00 | 30.67 | L | C |
| ATOM | 3931 | O | PRO | 112 | 104.936 | -28.166 | 22.353 | 1.00 | 31.28 | L | O |
| ATOM | 3932 | N | SER | 113 | 105.220 | -26.618 | 23.947 | 1.00 | 12.97 | L | N |
| ATOM | 3933 | CA | SER | 113 | 104.530 | -27.410 | 24.944 | 1.00 | 16.57 | L | C |
| ATOM | 3934 | CB | SER | 113 | 105.027 | -27.079 | 26.334 | 1.00 | 14.96 | L | C |
| ATOM | 3935 | OG | SER | 113 | 106.427 | -27.168 | 26.370 | 1.00 | 27.37 | L | O |
| ATOM | 3936 | C | SER | 113 | 103.099 | -26.913 | 24.815 | 1.00 | 15.10 | L | C |
| ATOM | 3937 | O | SER | 113 | 102.884 | -25.708 | 24.770 | 1.00 | 12.98 | L | O |
| ATOM | 3938 | N | VAL | 114 | 102.111 | -27.792 | 24.731 | 1.00 | 10.23 | L | N |
| ATOM | 3939 | CA | VAL | 114 | 100.766 | -27.258 | 24.630 | 1.00 | 9.98 | L | C |
| ATOM | 3940 | CB | VAL | 114 | 99.989 | -27.808 | 23.413 | 1.00 | 7.82 | L | C |
| ATOM | 3941 | CG1 | VAL | 114 | 100.921 | -27.972 | 22.212 | 1.00 | 4.17 | L | C |
| ATOM | 3942 | CG2 | VAL | 114 | 99.331 | -29.100 | 23.777 | 1.00 | 9.35 | L | C |

Fig. 19: A-55

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 3943 | C | VAL | 114 | 99.992 | -27.558 | 25.899 | 1.00 | 9.84 | L | C |
| ATOM | 3944 | O | VAL | 114 | 100.318 | -28.494 | 26.628 | 1.00 | 12.49 | L | O |
| ATOM | 3945 | N | PHE | 115 | 98.981 | -26.728 | 26.153 | 1.00 | 26.11 | L | N |
| ATOM | 3946 | CA | PHE | 115 | 98.109 | -26.840 | 27.318 | 1.00 | 30.12 | L | C |
| ATOM | 3947 | CB | PHE | 115 | 98.581 | -25.896 | 28.416 | 1.00 | 36.06 | L | C |
| ATOM | 3948 | CG | PHE | 115 | 100.030 | -26.015 | 28.706 | 1.00 | 35.84 | L | C |
| ATOM | 3949 | CD1 | PHE | 115 | 100.505 | -27.040 | 29.513 | 1.00 | 38.16 | L | C |
| ATOM | 3950 | CD2 | PHE | 115 | 100.935 | -25.146 | 28.115 | 1.00 | 34.45 | L | C |
| ATOM | 3951 | CE1 | PHE | 115 | 101.854 | -27.203 | 29.723 | 1.00 | 41.30 | L | C |
| ATOM | 3952 | CE2 | PHE | 115 | 102.287 | -25.302 | 28.319 | 1.00 | 38.56 | L | C |
| ATOM | 3953 | CZ | PHE | 115 | 102.749 | -26.335 | 29.126 | 1.00 | 39.82 | L | C |
| ATOM | 3954 | C | PHE | 115 | 96.727 | -26.410 | 26.873 | 1.00 | 32.06 | L | C |
| ATOM | 3955 | O | PHE | 115 | 96.590 | -25.543 | 26.017 | 1.00 | 32.56 | L | O |
| ATOM | 3956 | N | ILE | 116 | 95.694 | -27.018 | 27.432 | 1.00 | 24.34 | L | N |
| ATOM | 3957 | CA | ILE | 116 | 94.354 | -26.608 | 27.069 | 1.00 | 18.54 | L | C |
| ATOM | 3958 | CB | ILE | 116 | 93.606 | -27.735 | 26.309 | 1.00 | 15.62 | L | C |
| ATOM | 3959 | CG2 | ILE | 116 | 93.239 | -28.855 | 27.249 | 1.00 | 4.34 | L | C |
| ATOM | 3960 | CG1 | ILE | 116 | 92.377 | -27.145 | 25.615 | 1.00 | 12.45 | L | C |
| ATOM | 3961 | CD1 | ILE | 116 | 91.695 | -28.089 | 24.646 | 1.00 | 4.28 | L | C |
| ATOM | 3962 | C | ILE | 116 | 93.661 | -26.233 | 28.371 | 1.00 | 19.64 | L | C |
| ATOM | 3963 | O | ILE | 116 | 93.931 | -26.834 | 29.412 | 1.00 | 19.05 | L | O |
| ATOM | 3964 | N | PHE | 117 | 92.802 | -25.217 | 28.308 | 1.00 | 17.52 | L | N |
| ATOM | 3965 | CA | PHE | 117 | 92.066 | -24.715 | 29.475 | 1.00 | 21.17 | L | C |
| ATOM | 3966 | CB | PHE | 117 | 92.501 | -23.295 | 29.828 | 1.00 | 22.98 | L | C |
| ATOM | 3967 | CG | PHE | 117 | 93.922 | -23.177 | 30.280 | 1.00 | 26.62 | L | C |
| ATOM | 3968 | CD1 | PHE | 117 | 94.293 | -23.562 | 31.559 | 1.00 | 29.31 | L | C |
| ATOM | 3969 | CD2 | PHE | 117 | 94.882 | -22.653 | 29.433 | 1.00 | 28.01 | L | C |
| ATOM | 3970 | CE1 | PHE | 117 | 95.599 | -23.421 | 31.988 | 1.00 | 28.27 | L | C |
| ATOM | 3971 | CE2 | PHE | 117 | 96.186 | -22.511 | 29.854 | 1.00 | 26.58 | L | C |
| ATOM | 3972 | CZ | PHE | 117 | 96.550 | -22.895 | 31.134 | 1.00 | 28.58 | L | C |
| ATOM | 3973 | C | PHE | 117 | 90.585 | -24.642 | 29.194 | 1.00 | 24.71 | L | C |
| ATOM | 3974 | O | PHE | 117 | 90.167 | -23.964 | 28.261 | 1.00 | 29.18 | L | O |
| ATOM | 3975 | N | PRO | 118 | 89.768 | -25.323 | 30.007 | 1.00 | 23.78 | L | N |
| ATOM | 3976 | CD | PRO | 118 | 90.235 | -26.376 | 30.926 | 1.00 | 9.40 | L | C |
| ATOM | 3977 | CA | PRO | 118 | 88.300 | -25.354 | 29.883 | 1.00 | 26.26 | L | C |
| ATOM | 3978 | CB | PRO | 118 | 87.907 | -26.568 | 30.718 | 1.00 | 9.92 | L | C |
| ATOM | 3979 | CG | PRO | 118 | 89.159 | -27.404 | 30.763 | 1.00 | 12.26 | L | C |
| ATOM | 3980 | C | PRO | 118 | 87.660 | -24.081 | 30.455 | 1.00 | 29.72 | L | C |
| ATOM | 3981 | O | PRO | 118 | 88.231 | -23.440 | 31.338 | 1.00 | 31.19 | L | O |
| ATOM | 3982 | N | PRO | 119 | 86.464 | -23.699 | 29.966 | 1.00 | 9.50 | L | N |
| ATOM | 3983 | CD | PRO | 119 | 85.678 | -24.330 | 28.892 | 1.00 | 26.21 | L | C |
| ATOM | 3984 | CA | PRO | 119 | 85.787 | -22.493 | 30.479 | 1.00 | 9.82 | L | C |
| ATOM | 3985 | CB | PRO | 119 | 84.413 | -22.555 | 29.826 | 1.00 | 24.20 | L | C |
| ATOM | 3986 | CG | PRO | 119 | 84.703 | -23.219 | 28.519 | 1.00 | 27.52 | L | C |
| ATOM | 3987 | C | PRO | 119 | 85.682 | -22.566 | 32.001 | 1.00 | 15.21 | L | C |
| ATOM | 3988 | O | PRO | 119 | 85.463 | -23.630 | 32.561 | 1.00 | 17.89 | L | O |
| ATOM | 3989 | N | SER | 120 | 85.843 | -21.435 | 32.665 | 1.00 | 31.09 | L | N |
| ATOM | 3990 | CA | SER | 120 | 85.765 | -21.378 | 34.118 | 1.00 | 35.08 | L | C |
| ATOM | 3991 | CB | SER | 120 | 86.299 | -20.027 | 34.586 | 1.00 | 17.54 | L | C |
| ATOM | 3992 | OG | SER | 120 | 85.709 | -18.983 | 33.832 | 1.00 | 27.86 | L | O |
| ATOM | 3993 | C | SER | 120 | 84.334 | -21.550 | 34.623 | 1.00 | 35.73 | L | C |
| ATOM | 3994 | O | SER | 120 | 83.370 | -21.381 | 33.869 | 1.00 | 35.32 | L | O |
| ATOM | 3995 | N | ASP | 121 | 84.185 | -21.896 | 35.897 | 1.00 | 24.20 | L | N |
| ATOM | 3996 | CA | ASP | 121 | 82.842 | -22.015 | 36.465 | 1.00 | 27.07 | L | C |
| ATOM | 3997 | CB | ASP | 121 | 82.897 | -22.458 | 37.937 | 1.00 | 55.35 | L | C |
| ATOM | 3998 | CG | ASP | 121 | 83.160 | -23.950 | 38.101 | 1.00 | 60.98 | L | C |
| ATOM | 3999 | OD1 | ASP | 121 | 82.573 | -24.736 | 37.331 | 1.00 | 62.35 | L | O |
| ATOM | 4000 | OD2 | ASP | 121 | 83.934 | -24.337 | 39.008 | 1.00 | 63.66 | L | O |
| ATOM | 4001 | C | ASP | 121 | 82.194 | -20.627 | 36.384 | 1.00 | 26.11 | L | C |
| ATOM | 4002 | O | ASP | 121 | 81.053 | -20.474 | 35.941 | 1.00 | 23.12 | L | O |
| ATOM | 4003 | N | GLU | 122 | 82.954 | -19.617 | 36.794 | 1.00 | 48.87 | L | N |
| ATOM | 4004 | CA | GLU | 122 | 82.490 | -18.234 | 36.797 | 1.00 | 47.43 | L | C |
| ATOM | 4005 | CB | GLU | 122 | 83.596 | -17.328 | 37.348 | 1.00 | 56.26 | L | C |
| ATOM | 4006 | CG | GLU | 122 | 83.180 | -15.870 | 37.529 | 1.00 | 59.80 | L | C |
| ATOM | 4007 | CD | GLU | 122 | 84.328 | -14.966 | 37.984 | 1.00 | 63.49 | L | C |
| ATOM | 4008 | OE1 | GLU | 122 | 84.099 | -13.741 | 38.109 | 1.00 | 64.12 | L | O |
| ATOM | 4009 | OE2 | GLU | 122 | 85.453 | -15.472 | 38.213 | 1.00 | 63.98 | L | O |
| ATOM | 4010 | C | GLU | 122 | 82.018 | -17.703 | 35.434 | 1.00 | 47.22 | L | C |
| ATOM | 4011 | O | GLU | 122 | 80.884 | -17.232 | 35.303 | 1.00 | 45.96 | L | O |
| ATOM | 4012 | N | GLN | 123 | 82.881 | -17.774 | 34.424 | 1.00 | 34.52 | L | N |
| ATOM | 4013 | CA | GLN | 123 | 82.523 | -17.273 | 33.102 | 1.00 | 32.32 | L | C |
| ATOM | 4014 | CB | GLN | 123 | 83.643 | -17.511 | 32.097 | 1.00 | 23.68 | L | C |
| ATOM | 4015 | CG | GLN | 123 | 83.286 | -17.000 | 30.723 | 1.00 | 24.85 | L | C |

Fig. 19: A-56

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 4016 | CD | GLN | 123 | 84.089 | -17.644 | 29.635 | 1.00 | 26.94 | L | C |
| ATOM | 4017 | OE1 | GLN | 123 | 83.877 | -17.369 | 28.463 | 1.00 | 23.36 | L | O |
| ATOM | 4018 | NE2 | GLN | 123 | 85.017 | -18.511 | 30.010 | 1.00 | 24.66 | L | N |
| ATOM | 4019 | C | GLN | 123 | 81.256 | -17.909 | 32.565 | 1.00 | 32.32 | L | C |
| ATOM | 4020 | O | GLN | 123 | 80.424 | -17.233 | 31.969 | 1.00 | 29.27 | L | O |
| ATOM | 4021 | N | LEU | 124 | 81.128 | -19.218 | 32.745 | 1.00 | 36.22 | L | N |
| ATOM | 4022 | CA | LEU | 124 | 79.938 | -19.926 | 32.288 | 1.00 | 37.57 | L | C |
| ATOM | 4023 | CB | LEU | 124 | 80.075 | -21.425 | 32.570 | 1.00 | 20.16 | L | C |
| ATOM | 4024 | CG | LEU | 124 | 80.878 | -22.173 | 31.498 | 1.00 | 19.96 | L | C |
| ATOM | 4025 | CD1 | LEU | 124 | 81.099 | -23.623 | 31.892 | 1.00 | 15.21 | L | C |
| ATOM | 4026 | CD2 | LEU | 124 | 80.123 | -22.085 | 30.176 | 1.00 | 18.53 | L | C |
| ATOM | 4027 | C | LEU | 124 | 78.722 | -19.355 | 33.003 | 1.00 | 41.33 | L | C |
| ATOM | 4028 | O | LEU | 124 | 77.648 | -19.204 | 32.417 | 1.00 | 43.14 | L | O |
| ATOM | 4029 | N | LYS | 125 | 78.912 | -19.022 | 34.274 | 1.00 | 101.23 | L | N |
| ATOM | 4030 | CA | LYS | 125 | 77.856 | -18.441 | 35.090 | 1.00 | 102.45 | L | C |
| ATOM | 4031 | CB | LYS | 125 | 78.355 | -18.285 | 36.534 | 1.00 | 60.11 | L | C |
| ATOM | 4032 | CG | LYS | 125 | 77.286 | -18.376 | 37.612 | 1.00 | 62.95 | L | C |
| ATOM | 4033 | CD | LYS | 125 | 76.737 | -19.797 | 37.713 | 1.00 | 68.67 | L | C |
| ATOM | 4034 | CE | LYS | 125 | 75.726 | -19.942 | 38.847 | 1.00 | 73.14 | L | C |
| ATOM | 4035 | NZ | LYS | 125 | 75.101 | -21.299 | 38.895 | 1.00 | 74.11 | L | N |
| ATOM | 4036 | C | LYS | 125 | 77.545 | -17.065 | 34.494 | 1.00 | 104.22 | L | C |
| ATOM | 4037 | O | LYS | 125 | 77.004 | -16.195 | 35.168 | 1.00 | 105.97 | L | O |
| ATOM | 4038 | N | SER | 126 | 77.892 | -16.880 | 33.222 | 1.00 | 44.02 | L | N |
| ATOM | 4039 | CA | SER | 126 | 77.693 | -15.614 | 32.522 | 1.00 | 43.14 | L | C |
| ATOM | 4040 | CB | SER | 126 | 79.045 | -14.925 | 32.308 | 1.00 | 48.89 | L | C |
| ATOM | 4041 | OG | SER | 126 | 78.953 | -13.915 | 31.324 | 1.00 | 52.18 | L | O |
| ATOM | 4042 | C | SER | 126 | 76.995 | -15.769 | 31.176 | 1.00 | 41.22 | L | C |
| ATOM | 4043 | O | SER | 126 | 76.469 | -14.802 | 30.631 | 1.00 | 40.32 | L | O |
| ATOM | 4044 | N | GLY | 127 | 77.007 | -16.978 | 30.626 | 1.00 | 29.57 | L | N |
| ATOM | 4045 | CA | GLY | 127 | 76.340 | -17.190 | 29.355 | 1.00 | 30.30 | L | C |
| ATOM | 4046 | C | GLY | 127 | 77.266 | -17.332 | 28.168 | 1.00 | 29.68 | L | C |
| ATOM | 4047 | O | GLY | 127 | 76.818 | -17.391 | 27.022 | 1.00 | 30.41 | L | O |
| ATOM | 4048 | N | THR | 128 | 78.564 | -17.375 | 28.432 | 1.00 | 60.53 | L | N |
| ATOM | 4049 | CA | THR | 128 | 79.530 | -17.531 | 27.360 | 1.00 | 57.77 | L | C |
| ATOM | 4050 | CB | THR | 128 | 80.105 | -16.180 | 26.921 | 1.00 | 55.78 | L | C |
| ATOM | 4051 | OG1 | THR | 128 | 79.080 | -15.424 | 26.264 | 1.00 | 56.94 | L | O |
| ATOM | 4052 | CG2 | THR | 128 | 81.259 | -16.381 | 25.960 | 1.00 | 54.81 | L | C |
| ATOM | 4053 | C | THR | 128 | 80.643 | -18.434 | 27.830 | 1.00 | 56.24 | L | C |
| ATOM | 4054 | O | THR | 128 | 80.979 | -18.446 | 29.015 | 1.00 | 51.99 | L | O |
| ATOM | 4055 | N | ALA | 129 | 81.201 | -19.203 | 26.901 | 1.00 | 18.93 | L | N |
| ATOM | 4056 | CA | ALA | 129 | 82.275 | -20.125 | 27.232 | 1.00 | 17.83 | L | C |
| ATOM | 4057 | CB | ALA | 129 | 81.779 | -21.558 | 27.108 | 1.00 | 65.23 | L | C |
| ATOM | 4058 | C | ALA | 129 | 83.512 | -19.937 | 26.374 | 1.00 | 17.59 | L | C |
| ATOM | 4059 | O | ALA | 129 | 83.443 | -19.993 | 25.148 | 1.00 | 23.96 | L | O |
| ATOM | 4060 | N | SER | 130 | 84.652 | -19.729 | 27.020 | 1.00 | 24.31 | L | N |
| ATOM | 4061 | CA | SER | 130 | 85.905 | -19.560 | 26.298 | 1.00 | 19.76 | L | C |
| ATOM | 4062 | CB | SER | 130 | 86.565 | -18.256 | 26.741 | 1.00 | 18.21 | L | C |
| ATOM | 4063 | OG | SER | 130 | 85.724 | -17.142 | 26.477 | 1.00 | 20.32 | L | O |
| ATOM | 4064 | C | SER | 130 | 86.835 | -20.755 | 26.573 | 1.00 | 16.63 | L | C |
| ATOM | 4065 | O | SER | 130 | 87.037 | -21.141 | 27.732 | 1.00 | 19.43 | L | O |
| ATOM | 4066 | N | VAL | 131 | 87.370 | -21.371 | 25.521 | 1.00 | 11.62 | L | N |
| ATOM | 4067 | CA | VAL | 131 | 88.294 | -22.502 | 25.686 | 1.00 | 9.15 | L | C |
| ATOM | 4068 | CB | VAL | 131 | 87.848 | -23.743 | 24.872 | 1.00 | 17.04 | L | C |
| ATOM | 4069 | CG1 | VAL | 131 | 88.738 | -24.927 | 25.196 | 1.00 | 21.32 | L | C |
| ATOM | 4070 | CG2 | VAL | 131 | 86.413 | -24.081 | 25.180 | 1.00 | 16.62 | L | C |
| ATOM | 4071 | C | VAL | 131 | 89.647 | -22.030 | 25.156 | 1.00 | 9.42 | L | C |
| ATOM | 4072 | O | VAL | 131 | 89.731 | -21.557 | 24.025 | 1.00 | 13.02 | L | O |
| ATOM | 4073 | N | VAL | 132 | 90.704 | -22.146 | 25.956 | 1.00 | 21.24 | L | N |
| ATOM | 4074 | CA | VAL | 132 | 92.011 | -21.677 | 25.501 | 1.00 | 16.30 | L | C |
| ATOM | 4075 | CB | VAL | 132 | 92.573 | -20.538 | 26.414 | 1.00 | 43.77 | L | C |
| ATOM | 4076 | CG1 | VAL | 132 | 93.958 | -20.122 | 25.934 | 1.00 | 47.77 | L | C |
| ATOM | 4077 | CG2 | VAL | 132 | 91.645 | -19.324 | 26.393 | 1.00 | 44.24 | L | C |
| ATOM | 4078 | C | VAL | 132 | 93.081 | -22.743 | 25.374 | 1.00 | 17.14 | L | C |
| ATOM | 4079 | O | VAL | 132 | 93.372 | -23.482 | 26.320 | 1.00 | 14.49 | L | O |
| ATOM | 4080 | N | CYS | 133 | 93.662 | -22.793 | 24.178 | 1.00 | 23.86 | L | N |
| ATOM | 4081 | CA | CYS | 133 | 94.737 | -23.713 | 23.822 | 1.00 | 24.13 | L | C |
| ATOM | 4082 | C | CYS | 133 | 96.034 | -22.880 | 23.891 | 1.00 | 24.10 | L | C |
| ATOM | 4083 | O | CYS | 133 | 96.072 | -21.744 | 23.425 | 1.00 | 27.83 | L | O |
| ATOM | 4084 | CB | CYS | 133 | 94.486 | -24.219 | 22.399 | 1.00 | 19.56 | L | C |
| ATOM | 4085 | SG | CYS | 133 | 95.558 | -25.537 | 21.738 | 1.00 | 32.96 | L | S |
| ATOM | 4086 | N | LEU | 134 | 97.085 | -23.432 | 24.482 | 1.00 | 36.02 | L | N |
| ATOM | 4087 | CA | LEU | 134 | 98.343 | -22.709 | 24.591 | 1.00 | 34.35 | L | C |
| ATOM | 4088 | CB | LEU | 134 | 98.658 | -22.383 | 26.058 | 1.00 | 16.71 | L | C |

Fig. 19: A-57

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 4089 | CG | LEU | 134 | 100.079 | -21.843 | 26.376 | 1.00 | 12.52 | L | C |
| ATOM | 4090 | CD1 | LEU | 134 | 100.297 | -20.468 | 25.729 | 1.00 | 9.26 | L | C |
| ATOM | 4091 | CD2 | LEU | 134 | 100.275 | -21.746 | 27.892 | 1.00 | 9.75 | L | C |
| ATOM | 4092 | C | LEU | 134 | 99.532 | -23.457 | 24.001 | 1.00 | 33.88 | L | C |
| ATOM | 4093 | O | LEU | 134 | 99.820 | -24.595 | 24.378 | 1.00 | 33.96 | L | O |
| ATOM | 4094 | N | LEU | 135 | 100.206 | -22.802 | 23.060 | 1.00 | 23.69 | L | N |
| ATOM | 4095 | CA | LEU | 135 | 101.406 | -23.336 | 22.441 | 1.00 | 29.22 | L | C |
| ATOM | 4096 | CB | LEU | 135 | 101.353 | -23.150 | 20.926 | 1.00 | 1.87 | L | C |
| ATOM | 4097 | CG | LEU | 135 | 100.337 | -24.016 | 20.168 | 1.00 | 4.32 | L | C |
| ATOM | 4098 | CD1 | LEU | 135 | 98.962 | -23.751 | 20.672 | 1.00 | 5.12 | L | C |
| ATOM | 4099 | CD2 | LEU | 135 | 100.392 | -23.713 | 18.681 | 1.00 | 3.70 | L | C |
| ATOM | 4100 | C | LEU | 135 | 102.454 | -22.437 | 23.097 | 1.00 | 29.43 | L | C |
| ATOM | 4101 | O | LEU | 135 | 102.401 | -21.216 | 22.977 | 1.00 | 30.81 | L | O |
| ATOM | 4102 | N | ASN | 136 | 103.394 | -23.047 | 23.810 | 1.00 | 17.75 | L | N |
| ATOM | 4103 | CA | ASN | 136 | 104.393 | -22.299 | 24.550 | 1.00 | 20.05 | L | C |
| ATOM | 4104 | CB | ASN | 136 | 104.179 | -22.576 | 26.016 | 1.00 | 15.03 | L | C |
| ATOM | 4105 | CG | ASN | 136 | 104.905 | -21.615 | 26.885 | 1.00 | 19.57 | L | C |
| ATOM | 4106 | OD1 | ASN | 136 | 105.767 | -22.017 | 27.666 | 1.00 | 25.01 | L | O |
| ATOM | 4107 | ND2 | ASN | 136 | 104.569 | -20.327 | 26.769 | 1.00 | 19.54 | L | N |
| ATOM | 4108 | C | ASN | 136 | 105.856 | -22.526 | 24.212 | 1.00 | 18.78 | L | C |
| ATOM | 4109 | O | ASN | 136 | 106.283 | -23.651 | 23.963 | 1.00 | 17.25 | L | O |
| ATOM | 4110 | N | ASN | 137 | 106.619 | -21.436 | 24.240 | 1.00 | 28.11 | L | N |
| ATOM | 4111 | CA | ASN | 137 | 108.053 | -21.425 | 23.950 | 1.00 | 27.19 | L | C |
| ATOM | 4112 | CB | ASN | 137 | 108.869 | -21.844 | 25.173 | 1.00 | 13.82 | L | C |
| ATOM | 4113 | CG | ASN | 137 | 108.594 | -20.986 | 26.387 | 1.00 | 24.17 | L | C |
| ATOM | 4114 | OD1 | ASN | 137 | 108.027 | -19.901 | 26.281 | 1.00 | 19.30 | L | O |
| ATOM | 4115 | ND2 | ASN | 137 | 109.009 | -21.468 | 27.558 | 1.00 | 29.25 | L | N |
| ATOM | 4116 | C | ASN | 137 | 108.486 | -22.292 | 22.783 | 1.00 | 25.42 | L | C |
| ATOM | 4117 | O | ASN | 137 | 109.125 | -23.324 | 22.977 | 1.00 | 28.31 | L | O |
| ATOM | 4118 | N | PHE | 138 | 108.152 | -21.880 | 21.571 | 1.00 | 45.01 | L | N |
| ATOM | 4119 | CA | PHE | 138 | 108.557 | -22.652 | 20.412 | 1.00 | 41.21 | L | C |
| ATOM | 4120 | CB | PHE | 138 | 107.362 | -23.361 | 19.777 | 1.00 | 23.11 | L | C |
| ATOM | 4121 | CG | PHE | 138 | 106.230 | -22.452 | 19.442 | 1.00 | 20.89 | L | C |
| ATOM | 4122 | CD1 | PHE | 138 | 105.342 | -22.043 | 20.433 | 1.00 | 18.63 | L | C |
| ATOM | 4123 | CD2 | PHE | 138 | 106.055 | -21.993 | 18.137 | 1.00 | 19.93 | L | C |
| ATOM | 4124 | CE1 | PHE | 138 | 104.289 | -21.189 | 20.134 | 1.00 | 11.59 | L | C |
| ATOM | 4125 | CE2 | PHE | 138 | 105.010 | -21.138 | 17.818 | 1.00 | 16.52 | L | C |
| ATOM | 4126 | CZ | PHE | 138 | 104.118 | -20.730 | 18.818 | 1.00 | 14.07 | L | C |
| ATOM | 4127 | C | PHE | 138 | 109.248 | -21.794 | 19.369 | 1.00 | 36.81 | L | C |
| ATOM | 4128 | O | PHE | 138 | 109.456 | -20.594 | 19.559 | 1.00 | 35.37 | L | O |
| ATOM | 4129 | N | TYR | 139 | 109.606 | -22.437 | 18.267 | 1.00 | 17.70 | L | N |
| ATOM | 4130 | CA | TYR | 139 | 110.283 | -21.797 | 17.159 | 1.00 | 20.93 | L | C |
| ATOM | 4131 | CB | TYR | 139 | 111.660 | -21.300 | 17.579 | 1.00 | 31.56 | L | C |
| ATOM | 4132 | CG | TYR | 139 | 112.317 | -20.472 | 16.502 | 1.00 | 31.46 | L | C |
| ATOM | 4133 | CD1 | TYR | 139 | 112.207 | -19.083 | 16.502 | 1.00 | 26.49 | L | C |
| ATOM | 4134 | CE1 | TYR | 139 | 112.725 | -18.327 | 15.462 | 1.00 | 25.20 | L | C |
| ATOM | 4135 | CD2 | TYR | 139 | 112.974 | -21.083 | 15.428 | 1.00 | 25.20 | L | C |
| ATOM | 4136 | CE2 | TYR | 139 | 113.490 | -20.336 | 14.386 | 1.00 | 25.20 | L | C |
| ATOM | 4137 | CZ | TYR | 139 | 113.358 | -18.960 | 14.407 | 1.00 | 25.20 | L | C |
| ATOM | 4138 | OH | TYR | 139 | 113.820 | -18.216 | 13.353 | 1.00 | 28.00 | L | O |
| ATOM | 4139 | C | TYR | 139 | 110.447 | -22.917 | 16.166 | 1.00 | 20.32 | L | C |
| ATOM | 4140 | O | TYR | 139 | 110.798 | -24.022 | 16.550 | 1.00 | 25.25 | L | O |
| ATOM | 4141 | N | PRO | 140 | 110.223 | -22.662 | 14.876 | 1.00 | 34.32 | L | N |
| ATOM | 4142 | CD | PRO | 140 | 110.342 | -23.783 | 13.937 | 1.00 | 6.42 | L | C |
| ATOM | 4143 | CA | PRO | 140 | 109.824 | -21.443 | 14.171 | 1.00 | 30.02 | L | C |
| ATOM | 4144 | CB | PRO | 140 | 109.691 | -21.901 | 12.723 | 1.00 | 2.76 | L | C |
| ATOM | 4145 | CG | PRO | 140 | 110.570 | -23.070 | 12.643 | 1.00 | 4.42 | L | C |
| ATOM | 4146 | C | PRO | 140 | 108.502 | -20.939 | 14.685 | 1.00 | 31.53 | L | C |
| ATOM | 4147 | O | PRO | 140 | 107.830 | -21.612 | 15.466 | 1.00 | 29.36 | L | O |
| ATOM | 4148 | N | ARG | 141 | 108.119 | -19.764 | 14.203 | 1.00 | 22.83 | L | N |
| ATOM | 4149 | CA | ARG | 141 | 106.871 | -19.115 | 14.588 | 1.00 | 27.99 | L | C |
| ATOM | 4150 | CB | ARG | 141 | 106.931 | -17.657 | 14.148 | 1.00 | 21.70 | L | C |
| ATOM | 4151 | CG | ARG | 141 | 105.753 | -16.783 | 14.473 | 1.00 | 25.87 | L | C |
| ATOM | 4152 | CD | ARG | 141 | 106.157 | -15.358 | 14.129 | 1.00 | 37.20 | L | C |
| ATOM | 4153 | NE | ARG | 141 | 105.187 | -14.366 | 14.564 | 1.00 | 43.19 | L | N |
| ATOM | 4154 | CZ | ARG | 141 | 104.001 | -14.188 | 13.995 | 1.00 | 43.90 | L | C |
| ATOM | 4155 | NH1 | ARG | 141 | 103.642 | -14.941 | 12.960 | 1.00 | 39.57 | L | N |
| ATOM | 4156 | NH2 | ARG | 141 | 103.173 | -13.262 | 14.464 | 1.00 | 42.44 | L | N |
| ATOM | 4157 | C | ARG | 141 | 105.668 | -19.798 | 13.960 | 1.00 | 30.81 | L | C |
| ATOM | 4158 | O | ARG | 141 | 104.585 | -19.815 | 14.537 | 1.00 | 34.71 | L | O |
| ATOM | 4159 | N | GLU | 142 | 105.860 | -20.365 | 12.776 | 1.00 | 28.20 | L | N |
| ATOM | 4160 | CA | GLU | 142 | 104.756 | -21.013 | 12.091 | 1.00 | 24.33 | L | C |
| ATOM | 4161 | CB | GLU | 142 | 105.171 | -21.552 | 10.725 | 1.00 | 7.98 | L | C |

Fig. 19: A-58

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 4162 | CG | GLU | 142 | 105.741 | -20.523 | 9.781 | 1.00 | 19.00 | L | C |
| ATOM | 4163 | CD | GLU | 142 | 107.096 | -20.051 | 10.217 | 1.00 | 27.12 | L | C |
| ATOM | 4164 | OE1 | GLU | 142 | 107.152 | -18.970 | 10.837 | 1.00 | 31.02 | L | O |
| ATOM | 4165 | OE2 | GLU | 142 | 108.095 | -20.772 | 9.952 | 1.00 | 33.88 | L | O |
| ATOM | 4166 | C | GLU | 142 | 104.154 | -22.151 | 12.878 | 1.00 | 22.94 | L | C |
| ATOM | 4167 | O | GLU | 142 | 104.753 | -23.220 | 13.021 | 1.00 | 26.95 | L | O |
| ATOM | 4168 | N | ALA | 143 | 102.958 | -21.909 | 13.386 | 1.00 | 30.55 | L | N |
| ATOM | 4169 | CA | ALA | 143 | 102.238 | -22.914 | 14.130 | 1.00 | 32.81 | L | C |
| ATOM | 4170 | CB | ALA | 143 | 102.260 | -22.593 | 15.640 | 1.00 | 21.32 | L | C |
| ATOM | 4171 | C | ALA | 143 | 100.819 | -22.862 | 13.579 | 1.00 | 34.94 | L | C |
| ATOM | 4172 | O | ALA | 143 | 100.373 | -21.832 | 13.058 | 1.00 | 38.69 | L | O |
| ATOM | 4173 | N | LYS | 144 | 100.120 | -23.981 | 13.677 | 1.00 | 46.96 | L | N |
| ATOM | 4174 | CA | LYS | 144 | 98.761 | -24.047 | 13.197 | 1.00 | 49.64 | L | C |
| ATOM | 4175 | CB | LYS | 144 | 98.734 | -24.807 | 11.870 | 1.00 | 34.36 | L | C |
| ATOM | 4176 | CG | LYS | 144 | 97.631 | -24.370 | 10.922 | 1.00 | 44.31 | L | C |
| ATOM | 4177 | CD | LYS | 144 | 97.441 | -25.358 | 9.772 | 1.00 | 55.06 | L | C |
| ATOM | 4178 | CE | LYS | 144 | 96.888 | -26.699 | 10.279 | 1.00 | 57.35 | L | C |
| ATOM | 4179 | NZ | LYS | 144 | 96.807 | -27.761 | 9.225 | 1.00 | 58.76 | L | N |
| ATOM | 4180 | C | LYS | 144 | 97.934 | -24.771 | 14.266 | 1.00 | 52.97 | L | C |
| ATOM | 4181 | O | LYS | 144 | 98.340 | -25.822 | 14.775 | 1.00 | 51.55 | L | O |
| ATOM | 4182 | N | VAL | 145 | 96.791 | -24.194 | 14.630 | 1.00 | 15.87 | L | N |
| ATOM | 4183 | CA | VAL | 145 | 95.927 | -24.813 | 15.629 | 1.00 | 21.71 | L | C |
| ATOM | 4184 | CB | VAL | 145 | 95.790 | -23.937 | 16.905 | 1.00 | 8.53 | L | C |
| ATOM | 4185 | CG1 | VAL | 145 | 94.817 | -24.597 | 17.889 | 1.00 | 7.53 | L | C |
| ATOM | 4186 | CG2 | VAL | 145 | 97.151 | -23.769 | 17.570 | 1.00 | 8.28 | L | C |
| ATOM | 4187 | C | VAL | 145 | 94.536 | -25.074 | 15.073 | 1.00 | 25.32 | L | C |
| ATOM | 4188 | O | VAL | 145 | 93.909 | -24.193 | 14.497 | 1.00 | 27.49 | L | O |
| ATOM | 4189 | N | GLN | 146 | 94.055 | -26.296 | 15.231 | 1.00 | 39.17 | L | N |
| ATOM | 4190 | CA | GLN | 146 | 92.729 | -26.611 | 14.743 | 1.00 | 38.70 | L | C |
| ATOM | 4191 | CB | GLN | 146 | 92.798 | -27.679 | 13.653 | 1.00 | 72.09 | L | C |
| ATOM | 4192 | CG | GLN | 146 | 93.678 | -27.281 | 12.482 | 1.00 | 76.00 | L | C |
| ATOM | 4193 | CD | GLN | 146 | 93.630 | -28.276 | 11.339 | 1.00 | 75.94 | L | C |
| ATOM | 4194 | OE1 | GLN | 146 | 92.616 | -28.399 | 10.654 | 1.00 | 76.92 | L | O |
| ATOM | 4195 | NE2 | GLN | 146 | 94.730 | -28.997 | 11.130 | 1.00 | 77.33 | L | N |
| ATOM | 4196 | C | GLN | 146 | 91.880 | -27.094 | 15.904 | 1.00 | 37.70 | L | C |
| ATOM | 4197 | O | GLN | 146 | 92.302 | -27.965 | 16.667 | 1.00 | 34.46 | L | O |
| ATOM | 4198 | N | TRP | 147 | 90.699 | -26.498 | 16.048 | 1.00 | 30.86 | L | N |
| ATOM | 4199 | CA | TRP | 147 | 89.777 | -26.878 | 17.102 | 1.00 | 30.91 | L | C |
| ATOM | 4200 | CB | TRP | 147 | 88.947 | -25.687 | 17.556 | 1.00 | 36.68 | L | C |
| ATOM | 4201 | CG | TRP | 147 | 89.689 | -24.788 | 18.432 | 1.00 | 34.29 | L | C |
| ATOM | 4202 | CD2 | TRP | 147 | 89.927 | -24.969 | 19.825 | 1.00 | 32.37 | L | C |
| ATOM | 4203 | CE2 | TRP | 147 | 90.723 | -23.885 | 20.258 | 1.00 | 33.31 | L | C |
| ATOM | 4204 | CE3 | TRP | 147 | 89.552 | -25.943 | 20.752 | 1.00 | 31.13 | L | C |
| ATOM | 4205 | CD1 | TRP | 147 | 90.326 | -23.641 | 18.077 | 1.00 | 36.68 | L | C |
| ATOM | 4206 | NE1 | TRP | 147 | 90.951 | -23.086 | 19.168 | 1.00 | 33.41 | L | N |
| ATOM | 4207 | CZ2 | TRP | 147 | 91.150 | -23.747 | 21.587 | 1.00 | 31.66 | L | C |
| ATOM | 4208 | CZ3 | TRP | 147 | 89.977 | -25.808 | 22.073 | 1.00 | 33.39 | L | C |
| ATOM | 4209 | CH2 | TRP | 147 | 90.767 | -24.716 | 22.476 | 1.00 | 33.58 | L | C |
| ATOM | 4210 | C | TRP | 147 | 88.844 | -27.963 | 16.611 | 1.00 | 33.36 | L | C |
| ATOM | 4211 | O | TRP | 147 | 88.440 | -27.968 | 15.453 | 1.00 | 34.42 | L | O |
| ATOM | 4212 | N | LYS | 148 | 88.495 | -28.877 | 17.501 | 1.00 | 28.86 | L | N |
| ATOM | 4213 | CA | LYS | 148 | 87.609 | -29.958 | 17.147 | 1.00 | 29.96 | L | C |
| ATOM | 4214 | CB | LYS | 148 | 88.431 | -31.196 | 16.787 | 1.00 | 35.94 | L | C |
| ATOM | 4215 | CG | LYS | 148 | 88.353 | -31.585 | 15.320 | 1.00 | 39.31 | L | C |
| ATOM | 4216 | CD | LYS | 148 | 89.726 | -31.865 | 14.715 | 1.00 | 45.24 | L | C |
| ATOM | 4217 | CE | LYS | 148 | 90.421 | -33.078 | 15.337 | 1.00 | 45.54 | L | C |
| ATOM | 4218 | NZ | LYS | 148 | 91.826 | -33.267 | 14.818 | 1.00 | 44.96 | L | N |
| ATOM | 4219 | C | LYS | 148 | 86.712 | -30.227 | 18.340 | 1.00 | 32.40 | L | C |
| ATOM | 4220 | O | LYS | 148 | 87.197 | -30.505 | 19.438 | 1.00 | 31.51 | L | O |
| ATOM | 4221 | N | VAL | 149 | 85.404 | -30.124 | 18.118 | 1.00 | 22.85 | L | N |
| ATOM | 4222 | CA | VAL | 149 | 84.406 | -30.352 | 19.161 | 1.00 | 20.04 | L | C |
| ATOM | 4223 | CB | VAL | 149 | 83.453 | -29.167 | 19.269 | 1.00 | 1.90 | L | C |
| ATOM | 4224 | CG1 | VAL | 149 | 82.408 | -29.440 | 20.364 | 1.00 | 1.90 | L | C |
| ATOM | 4225 | CG2 | VAL | 149 | 84.242 | -27.899 | 19.563 | 1.00 | 1.90 | L | C |
| ATOM | 4226 | C | VAL | 149 | 83.580 | -31.605 | 18.862 | 1.00 | 23.24 | L | C |
| ATOM | 4227 | O | VAL | 149 | 82.835 | -31.642 | 17.883 | 1.00 | 24.43 | L | O |
| ATOM | 4228 | N | ASP | 150 | 83.679 | -32.611 | 19.731 | 1.00 | 18.00 | L | N |
| ATOM | 4229 | CA | ASP | 150 | 82.974 | -33.863 | 19.502 | 1.00 | 21.30 | L | C |
| ATOM | 4230 | CB | ASP | 150 | 81.464 | -33.661 | 19.459 | 1.00 | 45.33 | L | C |
| ATOM | 4231 | CG | ASP | 150 | 80.862 | -33.543 | 20.840 | 1.00 | 50.39 | L | C |
| ATOM | 4232 | OD1 | ASP | 150 | 81.334 | -34.248 | 21.760 | 1.00 | 51.76 | L | O |
| ATOM | 4233 | OD2 | ASP | 150 | 79.910 | -32.756 | 21.007 | 1.00 | 53.67 | L | O |
| ATOM | 4234 | C | ASP | 150 | 83.487 | -34.293 | 18.152 | 1.00 | 22.51 | L | C |

Fig. 19: A-59

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 4235 | O | ASP | 150 | 82.737 | -34.683 | 17.268 | 1.00 | 23.76 | L | O |
| ATOM | 4236 | N | ASN | 151 | 84.800 | -34.161 | 18.007 | 1.00 | 36.79 | L | N |
| ATOM | 4237 | CA | ASN | 151 | 85.493 | -34.524 | 16.789 | 1.00 | 39.62 | L | C |
| ATOM | 4238 | CB | ASN | 151 | 85.425 | -36.041 | 16.614 | 1.00 | 29.22 | L | C |
| ATOM | 4239 | CG | ASN | 151 | 86.220 | -36.776 | 17.683 | 1.00 | 38.58 | L | C |
| ATOM | 4240 | OD1 | ASN | 151 | 87.450 | -36.736 | 17.686 | 1.00 | 42.16 | L | O |
| ATOM | 4241 | ND2 | ASN | 151 | 85.522 | -37.430 | 18.608 | 1.00 | 39.63 | L | N |
| ATOM | 4242 | C | ASN | 151 | 84.985 | -33.778 | 15.557 | 1.00 | 37.90 | L | C |
| ATOM | 4243 | O | ASN | 151 | 85.224 | -34.183 | 14.425 | 1.00 | 41.98 | L | O |
| ATOM | 4244 | N | ALA | 152 | 84.293 | -32.672 | 15.793 | 1.00 | 26.76 | L | N |
| ATOM | 4245 | CA | ALA | 152 | 83.802 | -31.838 | 14.703 | 1.00 | 29.16 | L | C |
| ATOM | 4246 | CB | ALA | 152 | 82.421 | -31.261 | 15.034 | 1.00 | 1.87 | L | C |
| ATOM | 4247 | C | ALA | 152 | 84.801 | -30.698 | 14.501 | 1.00 | 30.47 | L | C |
| ATOM | 4248 | O | ALA | 152 | 84.940 | -29.813 | 15.355 | 1.00 | 32.16 | L | O |
| ATOM | 4249 | N | LEU | 153 | 85.502 | -30.724 | 13.375 | 1.00 | 37.66 | L | N |
| ATOM | 4250 | CA | LEU | 153 | 86.470 | -29.684 | 13.073 | 1.00 | 38.47 | L | C |
| ATOM | 4251 | CB | LEU | 153 | 87.021 | -29.896 | 11.656 | 1.00 | 33.69 | L | C |
| ATOM | 4252 | CG | LEU | 153 | 87.944 | -28.864 | 11.005 | 1.00 | 36.76 | L | C |
| ATOM | 4253 | CD1 | LEU | 153 | 87.112 | -27.705 | 10.466 | 1.00 | 35.54 | L | C |
| ATOM | 4254 | CD2 | LEU | 153 | 88.999 | -28.394 | 12.004 | 1.00 | 35.80 | L | C |
| ATOM | 4255 | C | LEU | 153 | 85.796 | -28.315 | 13.206 | 1.00 | 37.05 | L | C |
| ATOM | 4256 | O | LEU | 153 | 84.632 | -28.150 | 12.870 | 1.00 | 37.53 | L | O |
| ATOM | 4257 | N | GLN | 154 | 86.524 | -27.342 | 13.732 | 1.00 | 42.87 | L | N |
| ATOM | 4258 | CA | GLN | 154 | 85.984 | -26.006 | 13.885 | 1.00 | 41.76 | L | C |
| ATOM | 4259 | CB | GLN | 154 | 86.346 | -25.438 | 15.255 | 1.00 | 24.84 | L | C |
| ATOM | 4260 | CG | GLN | 154 | 85.653 | -26.133 | 16.403 | 1.00 | 25.94 | L | C |
| ATOM | 4261 | CD | GLN | 154 | 84.146 | -26.162 | 16.225 | 1.00 | 28.42 | L | C |
| ATOM | 4262 | OE1 | GLN | 154 | 83.495 | -25.115 | 16.127 | 1.00 | 30.98 | L | O |
| ATOM | 4263 | NE2 | GLN | 154 | 83.584 | -27.365 | 16.176 | 1.00 | 27.76 | L | N |
| ATOM | 4264 | C | GLN | 154 | 86.574 | -25.139 | 12.793 | 1.00 | 40.20 | L | C |
| ATOM | 4265 | O | GLN | 154 | 87.702 | -25.363 | 12.350 | 1.00 | 39.24 | L | O |
| ATOM | 4266 | N | SER | 155 | 85.813 | -24.146 | 12.359 | 1.00 | 42.27 | L | N |
| ATOM | 4267 | CA | SER | 155 | 86.269 | -23.257 | 11.306 | 1.00 | 44.34 | L | C |
| ATOM | 4268 | CB | SER | 155 | 85.770 | -23.768 | 9.952 | 1.00 | 47.84 | L | C |
| ATOM | 4269 | OG | SER | 155 | 86.319 | -23.035 | 8.872 | 1.00 | 49.98 | L | O |
| ATOM | 4270 | C | SER | 155 | 85.693 | -21.888 | 11.600 | 1.00 | 40.94 | L | C |
| ATOM | 4271 | O | SER | 155 | 86.208 | -20.864 | 11.160 | 1.00 | 39.18 | L | O |
| ATOM | 4272 | N | GLY | 156 | 84.621 | -21.877 | 12.374 | 1.00 | 21.85 | L | N |
| ATOM | 4273 | CA | GLY | 156 | 83.986 | -20.619 | 12.702 | 1.00 | 22.33 | L | C |
| ATOM | 4274 | C | GLY | 156 | 84.732 | -19.585 | 13.544 | 1.00 | 22.19 | L | C |
| ATOM | 4275 | O | GLY | 156 | 85.518 | -18.793 | 13.032 | 1.00 | 19.16 | L | O |
| ATOM | 4276 | N | ASN | 157 | 84.484 | -19.595 | 14.850 | 1.00 | 39.06 | L | N |
| ATOM | 4277 | CA | ASN | 157 | 85.088 | -18.595 | 15.697 | 1.00 | 40.50 | L | C |
| ATOM | 4278 | CB | ASN | 157 | 83.992 | -17.700 | 16.281 | 1.00 | 106.22 | L | C |
| ATOM | 4279 | CG | ASN | 157 | 83.201 | -16.977 | 15.200 | 1.00 | 109.22 | L | C |
| ATOM | 4280 | OD1 | ASN | 157 | 83.779 | -16.402 | 14.277 | 1.00 | 109.54 | L | O |
| ATOM | 4281 | ND2 | ASN | 157 | 81.874 | -16.999 | 15.313 | 1.00 | 114.95 | L | N |
| ATOM | 4282 | C | ASN | 157 | 86.059 | -18.997 | 16.790 | 1.00 | 41.01 | L | C |
| ATOM | 4283 | O | ASN | 157 | 85.713 | -19.566 | 17.827 | 1.00 | 40.41 | L | O |
| ATOM | 4284 | N | SER | 158 | 87.299 | -18.635 | 16.520 | 1.00 | 42.44 | L | N |
| ATOM | 4285 | CA | SER | 158 | 88.409 | -18.862 | 17.405 | 1.00 | 35.84 | L | C |
| ATOM | 4286 | CB | SER | 158 | 89.078 | -20.173 | 17.047 | 1.00 | 10.55 | L | C |
| ATOM | 4287 | OG | SER | 158 | 89.643 | -20.069 | 15.757 | 1.00 | 10.12 | L | O |
| ATOM | 4288 | C | SER | 158 | 89.326 | -17.691 | 17.059 | 1.00 | 34.29 | L | C |
| ATOM | 4289 | O | SER | 158 | 89.197 | -17.092 | 15.992 | 1.00 | 32.27 | L | O |
| ATOM | 4290 | N | GLN | 159 | 90.238 | -17.345 | 17.952 | 1.00 | 34.35 | L | N |
| ATOM | 4291 | CA | GLN | 159 | 91.133 | -16.250 | 17.652 | 1.00 | 31.73 | L | C |
| ATOM | 4292 | CB | GLN | 159 | 90.538 | -14.932 | 18.130 | 1.00 | 20.18 | L | C |
| ATOM | 4293 | CG | GLN | 159 | 89.399 | -14.413 | 17.266 | 1.00 | 21.46 | L | C |
| ATOM | 4294 | CD | GLN | 159 | 89.053 | -12.981 | 17.608 | 1.00 | 25.67 | L | C |
| ATOM | 4295 | OE1 | GLN | 159 | 88.796 | -12.658 | 18.762 | 1.00 | 28.88 | L | O |
| ATOM | 4296 | NE2 | GLN | 159 | 89.051 | -12.114 | 16.606 | 1.00 | 25.13 | L | N |
| ATOM | 4297 | C | GLN | 159 | 92.502 | -16.452 | 18.255 | 1.00 | 29.74 | L | C |
| ATOM | 4298 | O | GLN | 159 | 92.647 | -16.711 | 19.449 | 1.00 | 28.24 | L | O |
| ATOM | 4299 | N | GLU | 160 | 93.514 | -16.327 | 17.414 | 1.00 | 31.36 | L | N |
| ATOM | 4300 | CA | GLU | 160 | 94.872 | -16.510 | 17.865 | 1.00 | 24.49 | L | C |
| ATOM | 4301 | CB | GLU | 160 | 95.646 | -17.316 | 16.834 | 1.00 | 58.94 | L | C |
| ATOM | 4302 | CG | GLU | 160 | 94.977 | -18.617 | 16.476 | 1.00 | 59.06 | L | C |
| ATOM | 4303 | CD | GLU | 160 | 95.890 | -19.506 | 15.678 | 1.00 | 67.10 | L | C |
| ATOM | 4304 | OE1 | GLU | 160 | 95.463 | -20.619 | 15.285 | 1.00 | 71.37 | L | O |
| ATOM | 4305 | OE2 | GLU | 160 | 97.043 | -19.078 | 15.452 | 1.00 | 65.02 | L | O |
| ATOM | 4306 | C | GLU | 160 | 95.591 | -15.199 | 18.140 | 1.00 | 20.89 | L | C |
| ATOM | 4307 | O | GLU | 160 | 95.211 | -14.141 | 17.654 | 1.00 | 14.39 | L | O |

Fig. 19: A-60

```
ATOM   4308  N   SER   161      96.639 -15.293  18.941  1.00  19.35      L     N
ATOM   4309  CA  SER   161      97.456 -14.151  19.310  1.00  16.36      L     C
ATOM   4310  CB  SER   161      96.953 -13.486  20.597  1.00  26.12      L     C
ATOM   4311  OG  SER   161      97.935 -12.623  21.157  1.00  26.54      L     O
ATOM   4312  C   SER   161      98.811 -14.751  19.556  1.00  11.36      L     C
ATOM   4313  O   SER   161      98.934 -15.799  20.191  1.00  11.86      L     O
ATOM   4314  N   VAL   162      99.833 -14.086  19.053  1.00  21.19      L     N
ATOM   4315  CA  VAL   162     101.170 -14.592  19.215  1.00  22.81      L     C
ATOM   4316  CB  VAL   162     101.764 -14.965  17.832  1.00  29.37      L     C
ATOM   4317  CG1 VAL   162     101.449 -13.865  16.834  1.00  33.68      L     C
ATOM   4318  CG2 VAL   162     103.270 -15.178  17.933  1.00  33.85      L     C
ATOM   4319  C   VAL   162     101.997 -13.524  19.877  1.00  25.31      L     C
ATOM   4320  O   VAL   162     101.835 -12.349  19.566  1.00  32.55      L     O
ATOM   4321  N   THR   163     102.861 -13.928  20.805  1.00  22.97      L     N
ATOM   4322  CA  THR   163     103.735 -12.975  21.475  1.00  21.36      L     C
ATOM   4323  CB  THR   163     104.424 -13.567  22.719  1.00   4.31      L     C
ATOM   4324  OG1 THR   163     105.214 -14.705  22.342  1.00  10.67      L     O
ATOM   4325  CG2 THR   163     103.411 -13.966  23.748  1.00  -4.70      L     C
ATOM   4326  C   THR   163     104.842 -12.550  20.520  1.00  20.43      L     C
ATOM   4327  O   THR   163     104.880 -12.951  19.350  1.00  20.01      L     O
ATOM   4328  N   GLU   164     105.741 -11.722  21.022  1.00  16.64      L     N
ATOM   4329  CA  GLU   164     106.844 -11.283  20.211  1.00  24.33      L     C
ATOM   4330  CB  GLU   164     107.182  -9.828  20.515  1.00  53.60      L     C
ATOM   4331  CG  GLU   164     107.982  -9.187  19.415  1.00  64.34      L     C
ATOM   4332  CD  GLU   164     107.202  -9.144  18.126  1.00  70.19      L     C
ATOM   4333  OE1 GLU   164     106.337  -8.252  17.994  1.00  69.97      L     O
ATOM   4334  OE2 GLU   164     107.442 -10.011  17.257  1.00  73.61      L     O
ATOM   4335  C   GLU   164     107.989 -12.190  20.635  1.00  22.81      L     C
ATOM   4336  O   GLU   164     107.990 -12.697  21.765  1.00  25.48      L     O
ATOM   4337  N   GLN   165     108.948 -12.407  19.734  1.00  26.35      L     N
ATOM   4338  CA  GLN   165     110.100 -13.261  20.018  1.00  31.24      L     C
ATOM   4339  CB  GLN   165     111.181 -13.024  18.967  1.00  24.53      L     C
ATOM   4340  CG  GLN   165     111.927 -14.274  18.584  1.00  20.02      L     C
ATOM   4341  CD  GLN   165     112.911 -14.054  17.454  1.00  22.62      L     C
ATOM   4342  OE1 GLN   165     113.487 -15.005  16.930  1.00  23.83      L     O
ATOM   4343  NE2 GLN   165     113.118 -12.794  17.080  1.00  19.11      L     N
ATOM   4344  C   GLN   165     110.633 -12.941  21.412  1.00  35.11      L     C
ATOM   4345  O   GLN   165     110.857 -11.783  21.739  1.00  31.98      L     O
ATOM   4346  N   ASP   166     110.826 -13.963  22.236  1.00  20.85      L     N
ATOM   4347  CA  ASP   166     111.311 -13.741  23.592  1.00  27.22      L     C
ATOM   4348  CB  ASP   166     111.206 -15.030  24.402  1.00  40.40      L     C
ATOM   4349  CG  ASP   166     111.513 -14.813  25.872  1.00  48.39      L     C
ATOM   4350  OD1 ASP   166     112.706 -14.808  26.246  1.00  51.89      L     O
ATOM   4351  OD2 ASP   166     110.555 -14.631  26.655  1.00  52.06      L     O
ATOM   4352  C   ASP   166     112.741 -13.205  23.656  1.00  29.80      L     C
ATOM   4353  O   ASP   166     113.659 -13.787  23.079  1.00  33.62      L     O
ATOM   4354  N   SER   167     112.923 -12.098  24.371  1.00  40.62      L     N
ATOM   4355  CA  SER   167     114.238 -11.463  24.521  1.00  38.35      L     C
ATOM   4356  CB  SER   167     114.089 -10.092  25.191  1.00  42.38      L     C
ATOM   4357  OG  SER   167     113.564 -10.221  26.499  1.00  53.10      L     O
ATOM   4358  C   SER   167     115.229 -12.312  25.325  1.00  40.21      L     C
ATOM   4359  O   SER   167     116.373 -11.913  25.544  1.00  45.86      L     O
ATOM   4360  N   LYS   168     114.777 -13.475  25.782  1.00  39.00      L     N
ATOM   4361  CA  LYS   168     115.637 -14.383  26.527  1.00  40.59      L     C
ATOM   4362  CB  LYS   168     114.968 -14.809  27.837  1.00  73.78      L     C
ATOM   4363  CG  LYS   168     115.002 -13.726  28.916  1.00  80.02      L     C
ATOM   4364  CD  LYS   168     114.141 -12.523  28.554  1.00  89.23      L     C
ATOM   4365  CE  LYS   168     112.663 -12.805  28.778  1.00  96.32      L     C
ATOM   4366  NZ  LYS   168     112.355 -13.017  30.222  1.00  95.77      L     N
ATOM   4367  C   LYS   168     115.959 -15.597  25.650  1.00  39.39      L     C
ATOM   4368  O   LYS   168     117.046 -15.671  25.077  1.00  43.53      L     O
ATOM   4369  N   ASP   169     115.011 -16.522  25.506  1.00  18.93      L     N
ATOM   4370  CA  ASP   169     115.240 -17.716  24.686  1.00  15.08      L     C
ATOM   4371  CB  ASP   169     114.476 -18.913  25.262  1.00  29.81      L     C
ATOM   4372  CG  ASP   169     112.992 -18.648  25.407  1.00  32.60      L     C
ATOM   4373  OD1 ASP   169     112.397 -18.049  24.488  1.00  27.93      L     O
ATOM   4374  OD2 ASP   169     112.415 -19.054  26.441  1.00  29.85      L     O
ATOM   4375  C   ASP   169     114.914 -17.596  23.193  1.00  15.61      L     C
ATOM   4376  O   ASP   169     115.038 -18.571  22.459  1.00   9.73      L     O
ATOM   4377  N   SER   170     114.490 -16.418  22.747  1.00  28.98      L     N
ATOM   4378  CA  SER   170     114.170 -16.202  21.331  1.00  26.94      L     C
ATOM   4379  CB  SER   170     115.401 -16.487  20.433  1.00  15.64      L     C
ATOM   4380  OG  SER   170     116.466 -15.560  20.636  1.00  17.90      L     O
```

Fig. 19: A-61

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 4381 | C | SER | 170 | 112.995 | -17.042 | 20.825 | 1.00 | 25.42 | L | C |
| ATOM | 4382 | O | SER | 170 | 112.916 | -17.345 | 19.636 | 1.00 | 25.18 | L | O |
| ATOM | 4383 | N | THR | 171 | 112.071 | -17.411 | 21.702 | 1.00 | 22.07 | L | N |
| ATOM | 4384 | CA | THR | 171 | 110.946 | -18.222 | 21.247 | 1.00 | 22.16 | L | C |
| ATOM | 4385 | CB | THR | 171 | 110.658 | -19.406 | 22.212 | 1.00 | 16.53 | L | C |
| ATOM | 4386 | OG1 | THR | 171 | 110.127 | -18.911 | 23.452 | 1.00 | 18.93 | L | O |
| ATOM | 4387 | CG2 | THR | 171 | 111.939 | -20.191 | 22.471 | 1.00 | 18.13 | L | C |
| ATOM | 4388 | C | THR | 171 | 109.657 | -17.437 | 21.064 | 1.00 | 26.03 | L | C |
| ATOM | 4389 | O | THR | 171 | 109.601 | -16.235 | 21.327 | 1.00 | 31.48 | L | O |
| ATOM | 4390 | N | TYR | 172 | 108.633 | -18.147 | 20.596 | 1.00 | 7.82 | L | N |
| ATOM | 4391 | CA | TYR | 172 | 107.297 | -17.600 | 20.373 | 1.00 | 6.45 | L | C |
| ATOM | 4392 | CB | TYR | 172 | 106.934 | -17.706 | 18.894 | 1.00 | 43.65 | L | C |
| ATOM | 4393 | CG | TYR | 172 | 107.809 | -16.890 | 17.974 | 1.00 | 37.38 | L | C |
| ATOM | 4394 | CD1 | TYR | 172 | 107.652 | -15.507 | 17.865 | 1.00 | 32.97 | L | C |
| ATOM | 4395 | CE1 | TYR | 172 | 108.438 | -14.759 | 16.977 | 1.00 | 32.97 | L | C |
| ATOM | 4396 | CD2 | TYR | 172 | 108.776 | -17.508 | 17.181 | 1.00 | 37.97 | L | C |
| ATOM | 4397 | CE2 | TYR | 172 | 109.565 | -16.774 | 16.296 | 1.00 | 34.76 | L | C |
| ATOM | 4398 | CZ | TYR | 172 | 109.391 | -15.405 | 16.194 | 1.00 | 32.97 | L | C |
| ATOM | 4399 | OH | TYR | 172 | 110.163 | -14.703 | 15.294 | 1.00 | 32.97 | L | O |
| ATOM | 4400 | C | TYR | 172 | 106.255 | -18.364 | 21.212 | 1.00 | 6.45 | L | C |
| ATOM | 4401 | O | TYR | 172 | 106.431 | -19.539 | 21.528 | 1.00 | 9.78 | L | O |
| ATOM | 4402 | N | SER | 173 | 105.183 | -17.687 | 21.600 | 1.00 | 23.67 | L | N |
| ATOM | 4403 | CA | SER | 173 | 104.123 | -18.323 | 22.370 | 1.00 | 25.48 | L | C |
| ATOM | 4404 | CB | SER | 173 | 104.165 | -17.902 | 23.834 | 1.00 | 31.18 | L | C |
| ATOM | 4405 | OG | SER | 173 | 105.281 | -18.492 | 24.468 | 1.00 | 25.15 | L | O |
| ATOM | 4406 | C | SER | 173 | 102.836 | -17.886 | 21.728 | 1.00 | 26.94 | L | C |
| ATOM | 4407 | O | SER | 173 | 102.611 | -16.699 | 21.473 | 1.00 | 27.36 | L | O |
| ATOM | 4408 | N | LEU | 174 | 101.980 | -18.857 | 21.474 | 1.00 | 22.39 | L | N |
| ATOM | 4409 | CA | LEU | 174 | 100.734 | -18.593 | 20.791 | 1.00 | 25.49 | L | C |
| ATOM | 4410 | CB | LEU | 174 | 100.836 | -19.238 | 19.399 | 1.00 | 22.33 | L | C |
| ATOM | 4411 | CG | LEU | 174 | 99.682 | -19.165 | 18.422 | 1.00 | 13.39 | L | C |
| ATOM | 4412 | CD1 | LEU | 174 | 100.207 | -19.296 | 17.013 | 1.00 | 17.21 | L | C |
| ATOM | 4413 | CD2 | LEU | 174 | 98.663 | -20.257 | 18.769 | 1.00 | 10.23 | L | C |
| ATOM | 4414 | C | LEU | 174 | 99.510 | -19.075 | 21.562 | 1.00 | 27.64 | L | C |
| ATOM | 4415 | O | LEU | 174 | 99.542 | -20.111 | 22.229 | 1.00 | 30.82 | L | O |
| ATOM | 4416 | N | SER | 175 | 98.433 | -18.306 | 21.470 | 1.00 | 22.56 | L | N |
| ATOM | 4417 | CA | SER | 175 | 97.200 | -18.651 | 22.162 | 1.00 | 25.61 | L | C |
| ATOM | 4418 | CB | SER | 175 | 96.913 | -17.644 | 23.292 | 1.00 | 28.99 | L | C |
| ATOM | 4419 | OG | SER | 175 | 96.487 | -16.378 | 22.794 | 1.00 | 32.45 | L | O |
| ATOM | 4420 | C | SER | 175 | 96.009 | -18.693 | 21.214 | 1.00 | 29.48 | L | C |
| ATOM | 4421 | O | SER | 175 | 95.733 | -17.718 | 20.511 | 1.00 | 30.81 | L | O |
| ATOM | 4422 | N | SER | 176 | 95.316 | -19.829 | 21.181 | 1.00 | 31.99 | L | N |
| ATOM | 4423 | CA | SER | 176 | 94.125 | -19.957 | 20.346 | 1.00 | 32.77 | L | C |
| ATOM | 4424 | CB | SER | 176 | 94.154 | -21.247 | 19.514 | 1.00 | 10.71 | L | C |
| ATOM | 4425 | OG | SER | 176 | 93.247 | -21.176 | 18.421 | 1.00 | 10.34 | L | O |
| ATOM | 4426 | C | SER | 176 | 92.985 | -19.991 | 21.352 | 1.00 | 29.41 | L | C |
| ATOM | 4427 | O | SER | 176 | 93.042 | -20.712 | 22.350 | 1.00 | 29.56 | L | O |
| ATOM | 4428 | N | THR | 177 | 91.963 | -19.183 | 21.118 | 1.00 | 38.41 | L | N |
| ATOM | 4429 | CA | THR | 177 | 90.846 | -19.136 | 22.042 | 1.00 | 37.60 | L | C |
| ATOM | 4430 | CB | THR | 177 | 90.742 | -17.741 | 22.706 | 1.00 | 7.23 | L | C |
| ATOM | 4431 | OG1 | THR | 177 | 92.000 | -17.399 | 23.318 | 1.00 | 10.12 | L | O |
| ATOM | 4432 | CG2 | THR | 177 | 89.631 | -17.728 | 23.773 | 1.00 | 2.94 | L | C |
| ATOM | 4433 | C | THR | 177 | 89.551 | -19.455 | 21.311 | 1.00 | 35.94 | L | C |
| ATOM | 4434 | O | THR | 177 | 89.133 | -18.709 | 20.425 | 1.00 | 37.02 | L | O |
| ATOM | 4435 | N | LEU | 178 | 88.941 | -20.584 | 21.669 | 1.00 | 33.89 | L | N |
| ATOM | 4436 | CA | LEU | 178 | 87.682 | -21.015 | 21.072 | 1.00 | 32.44 | L | C |
| ATOM | 4437 | CB | LEU | 178 | 87.587 | -22.542 | 21.069 | 1.00 | 26.21 | L | C |
| ATOM | 4438 | CG | LEU | 178 | 86.291 | -23.170 | 20.539 | 1.00 | 27.24 | L | C |
| ATOM | 4439 | CD1 | LEU | 178 | 86.077 | -22.824 | 19.070 | 1.00 | 27.77 | L | C |
| ATOM | 4440 | CD2 | LEU | 178 | 86.367 | -24.683 | 20.730 | 1.00 | 15.35 | L | C |
| ATOM | 4441 | C | LEU | 178 | 86.552 | -20.412 | 21.901 | 1.00 | 32.70 | L | C |
| ATOM | 4442 | O | LEU | 178 | 86.476 | -20.589 | 23.120 | 1.00 | 29.14 | L | O |
| ATOM | 4443 | N | THR | 179 | 85.669 | -19.683 | 21.244 | 1.00 | 21.74 | L | N |
| ATOM | 4444 | CA | THR | 179 | 84.598 | -19.059 | 21.983 | 1.00 | 27.65 | L | C |
| ATOM | 4445 | CB | THR | 179 | 84.804 | -17.547 | 22.031 | 1.00 | 33.66 | L | C |
| ATOM | 4446 | OG1 | THR | 179 | 83.651 | -16.929 | 22.608 | 1.00 | 34.46 | L | O |
| ATOM | 4447 | CG2 | THR | 179 | 85.056 | -17.005 | 20.633 | 1.00 | 33.07 | L | C |
| ATOM | 4448 | C | THR | 179 | 83.223 | -19.377 | 21.430 | 1.00 | 32.00 | L | C |
| ATOM | 4449 | O | THR | 179 | 82.928 | -19.104 | 20.271 | 1.00 | 32.92 | L | O |
| ATOM | 4450 | N | LEU | 180 | 82.398 | -19.981 | 22.278 | 1.00 | 32.07 | L | N |
| ATOM | 4451 | CA | LEU | 180 | 81.035 | -20.349 | 21.922 | 1.00 | 33.73 | L | C |
| ATOM | 4452 | CB | LEU | 180 | 80.936 | -21.831 | 21.528 | 1.00 | 30.85 | L | C |
| ATOM | 4453 | CG | LEU | 180 | 82.059 | -22.804 | 21.881 | 1.00 | 33.56 | L | C |

Fig. 19: A-62

```
ATOM   4454  CD1 LEU   180      82.518 -22.589  23.309  1.00  36.03      L     C
ATOM   4455  CD2 LEU   180      81.552 -24.220  21.697  1.00  34.15      L     C
ATOM   4456  C   LEU   180      80.093 -20.062  23.084  1.00  37.58      L     C
ATOM   4457  O   LEU   180      80.526 -19.899  24.229  1.00  37.41      L     O
ATOM   4458  N   SER   181      78.801 -20.000  22.772  1.00  28.10      L     N
ATOM   4459  CA  SER   181      77.778 -19.711  23.770  1.00  31.26      L     C
ATOM   4460  CB  SER   181      76.433 -19.537  23.087  1.00  22.13      L     C
ATOM   4461  OG  SER   181      76.019 -20.764  22.513  1.00  25.39      L     O
ATOM   4462  C   SER   181      77.655 -20.802  24.815  1.00  33.74      L     C
ATOM   4463  O   SER   181      77.917 -21.978  24.533  1.00  33.98      L     O
ATOM   4464  N   LYS   182      77.247 -20.402  26.019  1.00  29.35      L     N
ATOM   4465  CA  LYS   182      77.060 -21.339  27.120  1.00  30.58      L     C
ATOM   4466  CB  LYS   182      76.375 -20.647  28.307  1.00  27.86      L     C
ATOM   4467  CG  LYS   182      76.341 -21.446  29.627  1.00  29.57      L     C
ATOM   4468  CD  LYS   182      74.912 -21.752  30.107  1.00  31.50      L     C
ATOM   4469  CE  LYS   182      74.863 -22.027  31.619  1.00  34.15      L     C
ATOM   4470  NZ  LYS   182      73.622 -22.756  32.099  1.00  38.40      L     N
ATOM   4471  C   LYS   182      76.167 -22.438  26.573  1.00  28.49      L     C
ATOM   4472  O   LYS   182      76.358 -23.618  26.878  1.00  20.36      L     O
ATOM   4473  N   ALA   183      75.206 -22.030  25.743  1.00  42.67      L     N
ATOM   4474  CA  ALA   183      74.252 -22.937  25.108  1.00  43.14      L     C
ATOM   4475  CB  ALA   183      73.319 -22.150  24.203  1.00  20.20      L     C
ATOM   4476  C   ALA   183      74.929 -24.053  24.313  1.00  42.26      L     C
ATOM   4477  O   ALA   183      74.645 -25.229  24.531  1.00  43.50      L     O
ATOM   4478  N   ASP   184      75.820 -23.691  23.395  1.00  37.65      L     N
ATOM   4479  CA  ASP   184      76.523 -24.692  22.587  1.00  39.98      L     C
ATOM   4480  CB  ASP   184      77.271 -24.023  21.434  1.00  60.24      L     C
ATOM   4481  CG  ASP   184      76.362 -23.219  20.545  1.00  66.97      L     C
ATOM   4482  OD1 ASP   184      75.360 -23.784  20.055  1.00  70.29      L     O
ATOM   4483  OD2 ASP   184      76.653 -22.023  20.335  1.00  70.50      L     O
ATOM   4484  C   ASP   184      77.519 -25.525  23.395  1.00  38.91      L     C
ATOM   4485  O   ASP   184      77.531 -26.753  23.308  1.00  36.50      L     O
ATOM   4486  N   TYR   185      78.362 -24.849  24.167  1.00  50.74      L     N
ATOM   4487  CA  TYR   185      79.352 -25.544  24.972  1.00  51.74      L     C
ATOM   4488  CB  TYR   185      80.011 -24.589  25.965  1.00  23.76      L     C
ATOM   4489  CG  TYR   185      81.104 -25.256  26.771  1.00  21.08      L     C
ATOM   4490  CD1 TYR   185      82.328 -25.552  26.192  1.00  16.43      L     C
ATOM   4491  CE1 TYR   185      83.332 -26.186  26.915  1.00  15.99      L     C
ATOM   4492  CD2 TYR   185      80.905 -25.613  28.104  1.00  17.64      L     C
ATOM   4493  CE2 TYR   185      81.902 -26.244  28.839  1.00  14.97      L     C
ATOM   4494  CZ  TYR   185      83.118 -26.526  28.235  1.00  14.93      L     C
ATOM   4495  OH  TYR   185      84.141 -27.119  28.944  1.00  16.56      L     O
ATOM   4496  C   TYR   185      78.729 -26.695  25.756  1.00  52.88      L     C
ATOM   4497  O   TYR   185      79.364 -27.728  25.978  1.00  52.42      L     O
ATOM   4498  N   GLU   186      77.484 -26.505  26.177  1.00  52.93      L     N
ATOM   4499  CA  GLU   186      76.787 -27.509  26.965  1.00  54.71      L     C
ATOM   4500  CB  GLU   186      75.643 -26.870  27.748  1.00  28.62      L     C
ATOM   4501  CG  GLU   186      76.067 -26.060  28.955  1.00  35.11      L     C
ATOM   4502  CD  GLU   186      74.876 -25.493  29.702  1.00  38.66      L     C
ATOM   4503  OE1 GLU   186      75.089 -24.850  30.746  1.00  41.21      L     O
ATOM   4504  OE2 GLU   186      73.725 -25.689  29.245  1.00  36.89      L     O
ATOM   4505  C   GLU   186      76.242 -28.694  26.190  1.00  52.40      L     C
ATOM   4506  O   GLU   186      76.029 -29.755  26.769  1.00  48.88      L     O
ATOM   4507  N   LYS   187      76.004 -28.538  24.895  1.00  35.74      L     N
ATOM   4508  CA  LYS   187      75.472 -29.662  24.147  1.00  37.64      L     C
ATOM   4509  CB  LYS   187      74.507 -29.173  23.057  1.00  53.22      L     C
ATOM   4510  CG  LYS   187      75.138 -28.512  21.849  1.00  54.27      L     C
ATOM   4511  CD  LYS   187      74.055 -27.941  20.930  1.00  53.80      L     C
ATOM   4512  CE  LYS   187      74.665 -27.203  19.740  1.00  49.76      L     C
ATOM   4513  NZ  LYS   187      73.707 -26.272  19.069  1.00  48.24      L     N
ATOM   4514  C   LYS   187      76.568 -30.553  23.549  1.00  36.73      L     C
ATOM   4515  O   LYS   187      76.287 -31.436  22.732  1.00  37.96      L     O
ATOM   4516  N   HIS   188      77.813 -30.339  23.972  1.00  23.77      L     N
ATOM   4517  CA  HIS   188      78.934 -31.124  23.468  1.00  21.36      L     C
ATOM   4518  CB  HIS   188      79.811 -30.257  22.562  1.00  41.13      L     C
ATOM   4519  CG  HIS   188      79.099 -29.774  21.338  1.00  42.53      L     C
ATOM   4520  CD2 HIS   188      78.800 -28.524  20.913  1.00  44.25      L     C
ATOM   4521  ND1 HIS   188      78.562 -30.633  20.405  1.00  41.45      L     N
ATOM   4522  CE1 HIS   188      77.961 -29.935  19.458  1.00  45.45      L     C
ATOM   4523  NE2 HIS   188      78.090 -28.652  19.743  1.00  43.75      L     N
ATOM   4524  C   HIS   188      79.743 -31.715  24.610  1.00  19.53      L     C
ATOM   4525  O   HIS   188      79.648 -31.253  25.751  1.00  19.70      L     O
ATOM   4526  N   LYS   189      80.521 -32.747  24.294  1.00  33.83      L     N
```

Fig. 19: A-63

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 4527 | CA | LYS | 189 | 81.334 | -33.445 | 25.281 | 1.00 | 33.86 | L | C |
| ATOM | 4528 | CB | LYS | 189 | 81.136 | -34.957 | 25.152 | 1.00 | 43.10 | L | C |
| ATOM | 4529 | CG | LYS | 189 | 79.898 | -35.516 | 25.815 | 1.00 | 47.03 | L | C |
| ATOM | 4530 | CD | LYS | 189 | 79.974 | -37.041 | 25.887 | 1.00 | 53.76 | L | C |
| ATOM | 4531 | CE | LYS | 189 | 79.997 | -37.680 | 24.505 | 1.00 | 59.30 | L | C |
| ATOM | 4532 | NZ | LYS | 189 | 78.694 | -37.545 | 23.794 | 1.00 | 59.64 | L | N |
| ATOM | 4533 | C | LYS | 189 | 82.831 | -33.155 | 25.201 | 1.00 | 33.18 | L | C |
| ATOM | 4534 | O | LYS | 189 | 83.435 | -32.657 | 26.155 | 1.00 | 36.85 | L | O |
| ATOM | 4535 | N | VAL | 190 | 83.435 | -33.482 | 24.069 | 1.00 | 39.67 | L | N |
| ATOM | 4536 | CA | VAL | 190 | 84.860 | -33.260 | 23.916 | 1.00 | 35.33 | L | C |
| ATOM | 4537 | CB | VAL | 190 | 85.516 | -34.439 | 23.214 | 1.00 | 33.71 | L | C |
| ATOM | 4538 | CG1 | VAL | 190 | 85.356 | -35.648 | 24.059 | 1.00 | 26.86 | L | C |
| ATOM | 4539 | CG2 | VAL | 190 | 84.880 | -34.657 | 21.855 | 1.00 | 36.79 | L | C |
| ATOM | 4540 | C | VAL | 190 | 85.249 | -31.992 | 23.170 | 1.00 | 35.17 | L | C |
| ATOM | 4541 | O | VAL | 190 | 84.656 | -31.641 | 22.141 | 1.00 | 36.62 | L | O |
| ATOM | 4542 | N | TYR | 191 | 86.256 | -31.319 | 23.718 | 1.00 | 27.65 | L | N |
| ATOM | 4543 | CA | TYR | 191 | 86.811 | -30.105 | 23.152 | 1.00 | 26.85 | L | C |
| ATOM | 4544 | CB | TYR | 191 | 86.554 | -28.934 | 24.095 | 1.00 | 16.61 | L | C |
| ATOM | 4545 | CG | TYR | 191 | 85.109 | -28.475 | 24.056 | 1.00 | 23.44 | L | C |
| ATOM | 4546 | CD1 | TYR | 191 | 84.654 | -27.650 | 23.030 | 1.00 | 27.57 | L | C |
| ATOM | 4547 | CE1 | TYR | 191 | 83.322 | -27.300 | 22.929 | 1.00 | 29.06 | L | C |
| ATOM | 4548 | CD2 | TYR | 191 | 84.178 | -28.937 | 24.991 | 1.00 | 24.37 | L | C |
| ATOM | 4549 | CE2 | TYR | 191 | 82.838 | -28.592 | 24.894 | 1.00 | 25.88 | L | C |
| ATOM | 4550 | CZ | TYR | 191 | 82.419 | -27.773 | 23.859 | 1.00 | 28.22 | L | C |
| ATOM | 4551 | OH | TYR | 191 | 81.097 | -27.419 | 23.745 | 1.00 | 30.91 | L | O |
| ATOM | 4552 | C | TYR | 191 | 88.295 | -30.381 | 23.010 | 1.00 | 28.07 | L | C |
| ATOM | 4553 | O | TYR | 191 | 88.946 | -30.821 | 23.960 | 1.00 | 29.13 | L | O |
| ATOM | 4554 | N | ALA | 192 | 88.837 | -30.159 | 21.822 | 1.00 | 17.93 | L | N |
| ATOM | 4555 | CA | ALA | 192 | 90.246 | -30.425 | 21.621 | 1.00 | 13.94 | L | C |
| ATOM | 4556 | CB | ALA | 192 | 90.424 | -31.850 | 21.160 | 1.00 | 12.32 | L | C |
| ATOM | 4557 | C | ALA | 192 | 90.921 | -29.489 | 20.640 | 1.00 | 14.27 | L | C |
| ATOM | 4558 | O | ALA | 192 | 90.271 | -28.885 | 19.784 | 1.00 | 14.89 | L | O |
| ATOM | 4559 | N | CYS | 193 | 92.234 | -29.362 | 20.787 | 1.00 | 20.91 | L | N |
| ATOM | 4560 | CA | CYS | 193 | 93.015 | -28.544 | 19.883 | 1.00 | 19.50 | L | C |
| ATOM | 4561 | C | CYS | 193 | 94.268 | -29.301 | 19.502 | 1.00 | 17.29 | L | C |
| ATOM | 4562 | O | CYS | 193 | 95.057 | -29.729 | 20.352 | 1.00 | 15.43 | L | O |
| ATOM | 4563 | CB | CYS | 193 | 93.361 | -27.183 | 20.490 | 1.00 | 44.80 | L | C |
| ATOM | 4564 | SG | CYS | 193 | 94.412 | -27.194 | 21.962 | 1.00 | 52.58 | L | S |
| ATOM | 4565 | N | GLU | 194 | 94.411 | -29.480 | 18.195 | 1.00 | 24.90 | L | N |
| ATOM | 4566 | CA | GLU | 194 | 95.522 | -30.193 | 17.600 | 1.00 | 25.90 | L | C |
| ATOM | 4567 | CB | GLU | 194 | 95.004 | -30.956 | 16.384 | 1.00 | 66.26 | L | C |
| ATOM | 4568 | CG | GLU | 194 | 95.979 | -31.887 | 15.718 | 1.00 | 77.97 | L | C |
| ATOM | 4569 | CD | GLU | 194 | 95.392 | -32.479 | 14.461 | 1.00 | 83.25 | L | C |
| ATOM | 4570 | OE1 | GLU | 194 | 95.276 | -31.738 | 13.462 | 1.00 | 80.00 | L | O |
| ATOM | 4571 | OE2 | GLU | 194 | 95.028 | -33.674 | 14.477 | 1.00 | 89.05 | L | O |
| ATOM | 4572 | C | GLU | 194 | 96.546 | -29.158 | 17.175 | 1.00 | 25.27 | L | C |
| ATOM | 4573 | O | GLU | 194 | 96.204 | -28.171 | 16.538 | 1.00 | 23.30 | L | O |
| ATOM | 4574 | N | VAL | 195 | 97.798 | -29.373 | 17.537 | 1.00 | 38.95 | L | N |
| ATOM | 4575 | CA | VAL | 195 | 98.850 | -28.443 | 17.168 | 1.00 | 34.83 | L | C |
| ATOM | 4576 | CB | VAL | 195 | 99.715 | -28.048 | 18.403 | 1.00 | 15.18 | L | C |
| ATOM | 4577 | CG1 | VAL | 195 | 100.911 | -27.210 | 17.971 | 1.00 | 11.26 | L | C |
| ATOM | 4578 | CG2 | VAL | 195 | 98.869 | -27.268 | 19.395 | 1.00 | 16.15 | L | C |
| ATOM | 4579 | C | VAL | 195 | 99.730 | -29.115 | 16.126 | 1.00 | 34.14 | L | C |
| ATOM | 4580 | O | VAL | 195 | 99.964 | -30.319 | 16.180 | 1.00 | 32.63 | L | O |
| ATOM | 4581 | N | THR | 196 | 100.190 | -28.340 | 15.157 | 1.00 | 43.12 | L | N |
| ATOM | 4582 | CA | THR | 196 | 101.063 | -28.876 | 14.135 | 1.00 | 42.44 | L | C |
| ATOM | 4583 | CB | THR | 196 | 100.411 | -28.867 | 12.764 | 1.00 | 26.65 | L | C |
| ATOM | 4584 | OG1 | THR | 196 | 99.001 | -28.673 | 12.909 | 1.00 | 36.35 | L | O |
| ATOM | 4585 | CG2 | THR | 196 | 100.671 | -30.180 | 12.067 | 1.00 | 28.65 | L | C |
| ATOM | 4586 | C | THR | 196 | 102.233 | -27.927 | 14.121 | 1.00 | 42.04 | L | C |
| ATOM | 4587 | O | THR | 196 | 102.049 | -26.710 | 14.053 | 1.00 | 37.83 | L | O |
| ATOM | 4588 | N | HIS | 197 | 103.437 | -28.479 | 14.186 | 1.00 | 32.41 | L | N |
| ATOM | 4589 | CA | HIS | 197 | 104.623 | -27.653 | 14.217 | 1.00 | 27.77 | L | C |
| ATOM | 4590 | CB | HIS | 197 | 104.867 | -27.172 | 15.651 | 1.00 | 21.71 | L | C |
| ATOM | 4591 | CG | HIS | 197 | 105.914 | -26.113 | 15.762 | 1.00 | 23.27 | L | C |
| ATOM | 4592 | CD2 | HIS | 197 | 105.817 | -24.761 | 15.753 | 1.00 | 17.64 | L | C |
| ATOM | 4593 | ND1 | HIS | 197 | 107.257 | -26.402 | 15.868 | 1.00 | 25.39 | L | N |
| ATOM | 4594 | CE1 | HIS | 197 | 107.944 | -25.274 | 15.923 | 1.00 | 22.67 | L | C |
| ATOM | 4595 | NE2 | HIS | 197 | 107.093 | -24.264 | 15.854 | 1.00 | 24.76 | L | N |
| ATOM | 4596 | C | HIS | 197 | 105.825 | -28.417 | 13.708 | 1.00 | 24.98 | L | C |
| ATOM | 4597 | O | HIS | 197 | 105.932 | -29.629 | 13.885 | 1.00 | 29.24 | L | O |
| ATOM | 4598 | N | GLN | 198 | 106.728 | -27.687 | 13.070 | 1.00 | 28.46 | L | N |
| ATOM | 4599 | CA | GLN | 198 | 107.944 | -28.252 | 12.515 | 1.00 | 26.49 | L | C |

Fig. 19: A-64

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 4600 | CB | GLN | 198 | 108.840 | -27.114 | 12.048 | 1.00 | 34.42 | L | C |
| ATOM | 4601 | CG | GLN | 198 | 110.091 | -27.549 | 11.333 | 1.00 | 36.17 | L | C |
| ATOM | 4602 | CD | GLN | 198 | 110.868 | -26.365 | 10.821 | 1.00 | 48.65 | L | C |
| ATOM | 4603 | OE1 | GLN | 198 | 110.286 | -25.414 | 10.299 | 1.00 | 57.22 | L | O |
| ATOM | 4604 | NE2 | GLN | 198 | 112.185 | -26.414 | 10.956 | 1.00 | 51.65 | L | N |
| ATOM | 4605 | C | GLN | 198 | 108.681 | -29.107 | 13.541 | 1.00 | 29.43 | L | C |
| ATOM | 4606 | O | GLN | 198 | 109.331 | -30.088 | 13.182 | 1.00 | 31.15 | L | O |
| ATOM | 4607 | N | GLY | 199 | 108.568 | -28.728 | 14.815 | 1.00 | 31.39 | L | N |
| ATOM | 4608 | CA | GLY | 199 | 109.234 | -29.452 | 15.887 | 1.00 | 36.65 | L | C |
| ATOM | 4609 | C | GLY | 199 | 108.465 | -30.636 | 16.444 | 1.00 | 39.08 | L | C |
| ATOM | 4610 | O | GLY | 199 | 108.880 | -31.244 | 17.425 | 1.00 | 43.81 | L | O |
| ATOM | 4611 | N | LEU | 200 | 107.339 | -30.961 | 15.823 | 1.00 | 25.48 | L | N |
| ATOM | 4612 | CA | LEU | 200 | 106.510 | -32.087 | 16.247 | 1.00 | 22.67 | L | C |
| ATOM | 4613 | CB | LEU | 200 | 105.094 | -31.597 | 16.570 | 1.00 | 31.49 | L | C |
| ATOM | 4614 | CG | LEU | 200 | 104.868 | -31.002 | 17.964 | 1.00 | 34.60 | L | C |
| ATOM | 4615 | CD1 | LEU | 200 | 106.036 | -30.149 | 18.361 | 1.00 | 37.97 | L | C |
| ATOM | 4616 | CD2 | LEU | 200 | 103.592 | -30.188 | 17.967 | 1.00 | 34.28 | L | C |
| ATOM | 4617 | C | LEU | 200 | 106.463 | -33.152 | 15.144 | 1.00 | 23.29 | L | C |
| ATOM | 4618 | O | LEU | 200 | 106.089 | -32.869 | 14.003 | 1.00 | 24.15 | L | O |
| ATOM | 4619 | N | SER | 201 | 106.860 | -34.372 | 15.499 | 1.00 | 21.11 | L | N |
| ATOM | 4620 | CA | SER | 201 | 106.886 | -35.503 | 14.570 | 1.00 | 24.08 | L | C |
| ATOM | 4621 | CB | SER | 201 | 107.367 | -36.747 | 15.311 | 1.00 | 27.13 | L | C |
| ATOM | 4622 | OG | SER | 201 | 106.702 | -36.875 | 16.561 | 1.00 | 28.99 | L | O |
| ATOM | 4623 | C | SER | 201 | 105.510 | -35.761 | 13.957 | 1.00 | 24.14 | L | C |
| ATOM | 4624 | O | SER | 201 | 105.392 | -36.267 | 12.835 | 1.00 | 25.49 | L | O |
| ATOM | 4625 | N | SER | 202 | 104.476 | -35.405 | 14.717 | 1.00 | 17.09 | L | N |
| ATOM | 4626 | CA | SER | 202 | 103.086 | -35.562 | 14.302 | 1.00 | 21.15 | L | C |
| ATOM | 4627 | CB | SER | 202 | 102.636 | -37.010 | 14.522 | 1.00 | 43.22 | L | C |
| ATOM | 4628 | OG | SER | 202 | 103.011 | -37.462 | 15.810 | 1.00 | 46.12 | L | O |
| ATOM | 4629 | C | SER | 202 | 102.265 | -34.603 | 15.155 | 1.00 | 21.60 | L | C |
| ATOM | 4630 | O | SER | 202 | 102.656 | -34.296 | 16.282 | 1.00 | 27.36 | L | O |
| ATOM | 4631 | N | PRO | 203 | 101.119 | -34.121 | 14.636 | 1.00 | 22.94 | L | N |
| ATOM | 4632 | CD | PRO | 203 | 100.457 | -34.478 | 13.368 | 1.00 | 32.35 | L | C |
| ATOM | 4633 | CA | PRO | 203 | 100.290 | -33.187 | 15.407 | 1.00 | 18.89 | L | C |
| ATOM | 4634 | CB | PRO | 203 | 98.971 | -33.177 | 14.643 | 1.00 | 26.47 | L | C |
| ATOM | 4635 | CG | PRO | 203 | 99.416 | -33.370 | 13.223 | 1.00 | 29.48 | L | C |
| ATOM | 4636 | C | PRO | 203 | 100.128 | -33.646 | 16.836 | 1.00 | 18.90 | L | C |
| ATOM | 4637 | O | PRO | 203 | 100.178 | -34.842 | 17.100 | 1.00 | 21.86 | L | O |
| ATOM | 4638 | N | VAL | 204 | 99.980 | -32.693 | 17.753 | 1.00 | 28.11 | L | N |
| ATOM | 4639 | CA | VAL | 204 | 99.794 | -32.996 | 19.172 | 1.00 | 29.99 | L | C |
| ATOM | 4640 | CB | VAL | 204 | 100.759 | -32.201 | 20.081 | 1.00 | 20.42 | L | C |
| ATOM | 4641 | CG1 | VAL | 204 | 100.254 | -32.204 | 21.512 | 1.00 | 20.30 | L | C |
| ATOM | 4642 | CG2 | VAL | 204 | 102.141 | -32.819 | 20.036 | 1.00 | 15.23 | L | C |
| ATOM | 4643 | C | VAL | 204 | 98.393 | -32.574 | 19.514 | 1.00 | 33.93 | L | C |
| ATOM | 4644 | O | VAL | 204 | 97.887 | -31.601 | 18.963 | 1.00 | 35.36 | L | O |
| ATOM | 4645 | N | THR | 205 | 97.755 | -33.293 | 20.422 | 1.00 | 45.34 | L | N |
| ATOM | 4646 | CA | THR | 205 | 96.402 | -32.933 | 20.787 | 1.00 | 46.97 | L | C |
| ATOM | 4647 | CB | THR | 205 | 95.386 | -33.896 | 20.137 | 1.00 | 14.48 | L | C |
| ATOM | 4648 | OG1 | THR | 205 | 95.275 | -33.587 | 18.747 | 1.00 | 10.44 | L | O |
| ATOM | 4649 | CG2 | THR | 205 | 94.013 | -33.761 | 20.769 | 1.00 | 11.16 | L | C |
| ATOM | 4650 | C | THR | 205 | 96.169 | -32.886 | 22.280 | 1.00 | 47.18 | L | C |
| ATOM | 4651 | O | THR | 205 | 96.596 | -33.763 | 23.032 | 1.00 | 49.19 | L | O |
| ATOM | 4652 | N | LYS | 206 | 95.513 | -31.822 | 22.709 | 1.00 | 22.09 | L | N |
| ATOM | 4653 | CA | LYS | 206 | 95.167 | -31.681 | 24.108 | 1.00 | 26.52 | L | C |
| ATOM | 4654 | CB | LYS | 206 | 95.791 | -30.422 | 24.710 | 1.00 | 41.08 | L | C |
| ATOM | 4655 | CG | LYS | 206 | 97.208 | -30.641 | 25.215 | 1.00 | 44.88 | L | C |
| ATOM | 4656 | CD | LYS | 206 | 97.269 | -31.688 | 26.312 | 1.00 | 47.36 | L | C |
| ATOM | 4657 | CE | LYS | 206 | 98.654 | -31.760 | 26.957 | 1.00 | 49.27 | L | C |
| ATOM | 4658 | NZ | LYS | 206 | 99.723 | -32.144 | 25.997 | 1.00 | 50.40 | L | N |
| ATOM | 4659 | C | LYS | 206 | 93.653 | -31.602 | 24.100 | 1.00 | 29.29 | L | C |
| ATOM | 4660 | O | LYS | 206 | 93.063 | -30.939 | 23.246 | 1.00 | 34.45 | L | O |
| ATOM | 4661 | N | SER | 207 | 93.026 | -32.304 | 25.033 | 1.00 | 32.39 | L | N |
| ATOM | 4662 | CA | SER | 207 | 91.578 | -32.324 | 25.083 | 1.00 | 29.18 | L | C |
| ATOM | 4663 | CB | SER | 207 | 91.046 | -33.364 | 24.080 | 1.00 | 31.23 | L | C |
| ATOM | 4664 | OG | SER | 207 | 91.613 | -34.655 | 24.294 | 1.00 | 31.62 | L | O |
| ATOM | 4665 | C | SER | 207 | 91.039 | -32.624 | 26.476 | 1.00 | 28.78 | L | C |
| ATOM | 4666 | O | SER | 207 | 91.798 | -32.938 | 27.397 | 1.00 | 29.47 | L | O |
| ATOM | 4667 | N | PHE | 208 | 89.719 | -32.517 | 26.606 | 1.00 | 33.89 | L | N |
| ATOM | 4668 | CA | PHE | 208 | 89.013 | -32.777 | 27.852 | 1.00 | 39.79 | L | C |
| ATOM | 4669 | CB | PHE | 208 | 89.217 | -31.615 | 28.842 | 1.00 | 17.06 | L | C |
| ATOM | 4670 | CG | PHE | 208 | 88.662 | -30.300 | 28.353 | 1.00 | 14.11 | L | C |
| ATOM | 4671 | CD1 | PHE | 208 | 89.409 | -29.482 | 27.499 | 1.00 | 18.84 | L | C |
| ATOM | 4672 | CD2 | PHE | 208 | 87.376 | -29.906 | 28.690 | 1.00 | 11.57 | L | C |

Fig. 19: A-65

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 4673 | CE1 | PHE | 208 | 88.879 | -28.298 | 26.990 | 1.00 | 19.93 | L | C |
| ATOM | 4674 | CE2 | PHE | 208 | 86.846 | -28.729 | 28.182 | 1.00 | 14.34 | L | C |
| ATOM | 4675 | CZ | PHE | 208 | 87.602 | -27.925 | 27.330 | 1.00 | 20.99 | L | C |
| ATOM | 4676 | C | PHE | 208 | 87.536 | -32.873 | 27.472 | 1.00 | 45.59 | L | C |
| ATOM | 4677 | O | PHE | 208 | 87.168 | -32.576 | 26.335 | 1.00 | 47.78 | L | O |
| ATOM | 4678 | N | ASN | 209 | 86.703 | -33.293 | 28.420 | 1.00 | 24.67 | L | N |
| ATOM | 4679 | CA | ASN | 209 | 85.257 | -33.398 | 28.213 | 1.00 | 28.33 | L | C |
| ATOM | 4680 | CB | ASN | 209 | 84.751 | -34.785 | 28.623 | 1.00 | 27.05 | L | C |
| ATOM | 4681 | CG | ASN | 209 | 85.664 | -35.913 | 28.172 | 1.00 | 33.97 | L | C |
| ATOM | 4682 | OD1 | ASN | 209 | 85.777 | -36.941 | 28.841 | 1.00 | 34.19 | L | O |
| ATOM | 4683 | ND2 | ASN | 209 | 86.304 | -35.732 | 27.031 | 1.00 | 37.01 | L | N |
| ATOM | 4684 | C | ASN | 209 | 84.630 | -32.370 | 29.160 | 1.00 | 29.95 | L | C |
| ATOM | 4685 | O | ASN | 209 | 85.203 | -32.108 | 30.218 | 1.00 | 31.18 | L | O |
| ATOM | 4686 | N | ARG | 210 | 83.473 | -31.800 | 28.805 | 1.00 | 15.88 | L | N |
| ATOM | 4687 | CA | ARG | 210 | 82.810 | -30.829 | 29.687 | 1.00 | 19.72 | L | C |
| ATOM | 4688 | CB | ARG | 210 | 81.337 | -30.721 | 29.371 | 1.00 | 31.19 | L | C |
| ATOM | 4689 | CG | ARG | 210 | 81.027 | -29.666 | 28.361 | 1.00 | 32.77 | L | C |
| ATOM | 4690 | CD | ARG | 210 | 79.655 | -29.104 | 28.627 | 1.00 | 36.35 | L | C |
| ATOM | 4691 | NE | ARG | 210 | 78.656 | -30.166 | 28.633 | 1.00 | 41.72 | L | N |
| ATOM | 4692 | CZ | ARG | 210 | 77.502 | -30.095 | 29.282 | 1.00 | 45.49 | L | C |
| ATOM | 4693 | NH1 | ARG | 210 | 77.204 | -29.008 | 29.981 | 1.00 | 46.04 | L | N |
| ATOM | 4694 | NH2 | ARG | 210 | 76.655 | -31.112 | 29.232 | 1.00 | 47.73 | L | N |
| ATOM | 4695 | C | ARG | 210 | 82.964 | -31.252 | 31.137 | 1.00 | 22.05 | L | C |
| ATOM | 4696 | O | ARG | 210 | 82.962 | -32.440 | 31.428 | 1.00 | 23.93 | L | O |
| ATOM | 4697 | N | GLY | 211 | 83.096 | -30.291 | 32.048 | 1.00 | 53.99 | L | N |
| ATOM | 4698 | CA | GLY | 211 | 83.297 | -30.638 | 33.447 | 1.00 | 53.99 | L | C |
| ATOM | 4699 | C | GLY | 211 | 84.740 | -31.088 | 33.630 | 1.00 | 53.99 | L | C |
| ATOM | 4700 | O | GLY | 211 | 85.665 | -30.312 | 33.387 | 1.00 | 53.99 | L | O |
| ATOM | 4701 | N | GLU | 212 | 84.942 | -32.336 | 34.046 | 1.00 | 80.95 | L | N |
| ATOM | 4702 | CA | GLU | 212 | 86.287 | -32.890 | 34.236 | 1.00 | 80.95 | L | C |
| ATOM | 4703 | CB | GLU | 212 | 86.995 | -33.004 | 32.871 | 1.00 | 34.07 | L | C |
| ATOM | 4704 | CG | GLU | 212 | 88.259 | -33.888 | 32.849 | 1.00 | 34.07 | L | C |
| ATOM | 4705 | CD | GLU | 212 | 88.691 | -34.311 | 31.435 | 1.00 | 34.07 | L | C |
| ATOM | 4706 | OE1 | GLU | 212 | 89.803 | -34.863 | 31.296 | 1.00 | 34.07 | L | O |
| ATOM | 4707 | OE2 | GLU | 212 | 87.923 | -34.113 | 30.468 | 1.00 | 34.07 | L | O |
| ATOM | 4708 | C | GLU | 212 | 87.134 | -32.080 | 35.227 | 1.00 | 80.95 | L | C |
| ATOM | 4709 | O | GLU | 212 | 86.690 | -31.043 | 35.732 | 1.00 | 80.95 | L | O |
| ATOM | 4710 | N | CYS | 213 | 88.341 | -32.566 | 35.516 | 1.00 | 81.74 | L | N |
| ATOM | 4711 | CA | CYS | 213 | 89.243 | -31.893 | 36.450 | 1.00 | 81.74 | L | C |
| ATOM | 4712 | CB | CYS | 213 | 88.990 | -32.374 | 37.883 | 1.00 | 54.42 | L | C |
| ATOM | 4713 | SG | CYS | 213 | 87.479 | -31.701 | 38.656 | 1.00 | 54.42 | L | S |
| ATOM | 4714 | C | CYS | 213 | 90.715 | -32.123 | 36.095 | 1.00 | 81.74 | L | C |
| ATOM | 4715 | O | CYS | 213 | 90.996 | -32.758 | 35.051 | 1.00 | 81.74 | L | O |
| ATOM | 4716 | OXT | CYS | 213 | 91.581 | -31.647 | 36.863 | 1.00 | 72.88 | L | O |
| ATOM | 4717 | MN | MN | 400 | 117.831 | 24.682 | 6.345 | 1.00 | 34.24 | M | |
| ATOM | 4718 | CB | THR | 145 | 114.226 | 73.843 | 15.327 | 1.00 | 72.71 | B | C |
| ATOM | 4719 | OG1 | THR | 145 | 113.673 | 74.174 | 16.611 | 1.00 | 72.71 | B | O |
| ATOM | 4720 | CG2 | THR | 145 | 114.208 | 75.069 | 14.426 | 1.00 | 72.71 | B | C |
| ATOM | 4721 | C | THR | 145 | 113.665 | 71.399 | 15.485 | 1.00 | 109.74 | B | C |
| ATOM | 4722 | O | THR | 145 | 113.590 | 70.290 | 14.948 | 1.00 | 110.14 | B | O |
| ATOM | 4723 | N | THR | 145 | 111.957 | 72.996 | 14.632 | 1.00 | 108.12 | B | N |
| ATOM | 4724 | CA | THR | 145 | 113.414 | 72.677 | 14.686 | 1.00 | 107.72 | B | C |
| ATOM | 4725 | N | GLN | 146 | 113.963 | 71.561 | 16.769 | 1.00 | 79.22 | B | N |
| ATOM | 4726 | CA | GLN | 146 | 114.224 | 70.425 | 17.633 | 1.00 | 77.37 | B | C |
| ATOM | 4727 | CB | GLN | 146 | 115.554 | 70.620 | 18.378 | 1.00 | 80.28 | B | C |
| ATOM | 4728 | CG | GLN | 146 | 115.640 | 71.886 | 19.208 | 1.00 | 80.28 | B | C |
| ATOM | 4729 | CD | GLN | 146 | 116.952 | 72.001 | 19.955 | 1.00 | 80.28 | B | C |
| ATOM | 4730 | OE1 | GLN | 146 | 117.150 | 72.929 | 20.742 | 1.00 | 80.28 | B | O |
| ATOM | 4731 | NE2 | GLN | 146 | 117.858 | 71.059 | 19.712 | 1.00 | 80.28 | B | N |
| ATOM | 4732 | C | GLN | 146 | 113.077 | 70.200 | 18.620 | 1.00 | 77.79 | B | C |
| ATOM | 4733 | O | GLN | 146 | 112.818 | 71.018 | 19.511 | 1.00 | 79.65 | B | O |
| ATOM | 4734 | N | LEU | 147 | 112.383 | 69.081 | 18.432 | 1.00 | 43.47 | B | N |
| ATOM | 4735 | CA | LEU | 147 | 111.265 | 68.710 | 19.288 | 1.00 | 42.60 | B | C |
| ATOM | 4736 | CB | LEU | 147 | 109.936 | 68.755 | 18.525 | 1.00 | 51.95 | B | C |
| ATOM | 4737 | CG | LEU | 147 | 109.450 | 69.952 | 17.707 | 1.00 | 52.14 | B | C |
| ATOM | 4738 | CD1 | LEU | 147 | 110.464 | 70.296 | 16.632 | 1.00 | 47.35 | B | C |
| ATOM | 4739 | CD2 | LEU | 147 | 108.114 | 69.607 | 17.060 | 1.00 | 51.99 | B | C |
| ATOM | 4740 | C | LEU | 147 | 111.461 | 67.281 | 19.756 | 1.00 | 41.58 | B | C |
| ATOM | 4741 | O | LEU | 147 | 112.077 | 66.470 | 19.058 | 1.00 | 42.88 | B | O |
| ATOM | 4742 | N | ASP | 148 | 110.944 | 66.988 | 20.945 | 1.00 | 31.29 | B | N |
| ATOM | 4743 | CA | ASP | 148 | 110.974 | 65.640 | 21.493 | 1.00 | 28.75 | B | C |
| ATOM | 4744 | CB | ASP | 148 | 111.394 | 65.642 | 22.960 | 1.00 | 32.78 | B | C |
| ATOM | 4745 | CG | ASP | 148 | 112.897 | 65.718 | 23.133 | 1.00 | 32.40 | B | C |

Fig. 19: A-66

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 4746 | OD1 | ASP | 148 | 113.366 | 65.715 | 24.290 | 1.00 | 31.51 | B | O |
| ATOM | 4747 | OD2 | ASP | 148 | 113.616 | 65.777 | 22.116 | 1.00 | 30.58 | B | O |
| ATOM | 4748 | C | ASP | 148 | 109.526 | 65.181 | 21.358 | 1.00 | 25.13 | B | C |
| ATOM | 4749 | O | ASP | 148 | 108.664 | 65.583 | 22.128 | 1.00 | 24.43 | B | O |
| ATOM | 4750 | N | ILE | 149 | 109.260 | 64.368 | 20.345 | 1.00 | 21.33 | B | N |
| ATOM | 4751 | CA | ILE | 149 | 107.918 | 63.885 | 20.105 | 1.00 | 20.27 | B | C |
| ATOM | 4752 | CB | ILE | 149 | 107.610 | 63.880 | 18.605 | 1.00 | 13.57 | B | C |
| ATOM | 4753 | CG2 | ILE | 149 | 106.140 | 63.573 | 18.378 | 1.00 | 8.58 | B | C |
| ATOM | 4754 | CG1 | ILE | 149 | 107.932 | 65.234 | 17.998 | 1.00 | 9.29 | B | C |
| ATOM | 4755 | CD1 | ILE | 149 | 107.697 | 65.263 | 16.508 | 1.00 | 12.04 | B | C |
| ATOM | 4756 | C | ILE | 149 | 107.723 | 62.464 | 20.629 | 1.00 | 21.92 | B | C |
| ATOM | 4757 | O | ILE | 149 | 108.507 | 61.563 | 20.315 | 1.00 | 22.32 | B | O |
| ATOM | 4758 | N | VAL | 150 | 106.680 | 62.271 | 21.433 | 1.00 | 32.56 | B | N |
| ATOM | 4759 | CA | VAL | 150 | 106.357 | 60.950 | 21.956 | 1.00 | 34.12 | B | C |
| ATOM | 4760 | CB | VAL | 150 | 106.256 | 60.940 | 23.492 | 1.00 | 12.90 | B | C |
| ATOM | 4761 | CG1 | VAL | 150 | 105.775 | 59.579 | 23.967 | 1.00 | 15.09 | B | C |
| ATOM | 4762 | CG2 | VAL | 150 | 107.620 | 61.256 | 24.110 | 1.00 | 14.71 | B | C |
| ATOM | 4763 | C | VAL | 150 | 105.001 | 60.604 | 21.381 | 1.00 | 31.68 | B | C |
| ATOM | 4764 | O | VAL | 150 | 104.057 | 61.380 | 21.523 | 1.00 | 29.83 | B | O |
| ATOM | 4765 | N | ILE | 151 | 104.904 | 59.459 | 20.714 | 1.00 | 36.82 | B | N |
| ATOM | 4766 | CA | ILE | 151 | 103.640 | 59.037 | 20.115 | 1.00 | 35.62 | B | C |
| ATOM | 4767 | CB | ILE | 151 | 103.862 | 58.436 | 18.709 | 1.00 | 31.63 | B | C |
| ATOM | 4768 | CG2 | ILE | 151 | 102.537 | 58.084 | 18.081 | 1.00 | 27.99 | B | C |
| ATOM | 4769 | CG1 | ILE | 151 | 104.582 | 59.454 | 17.817 | 1.00 | 30.05 | B | C |
| ATOM | 4770 | CD1 | ILE | 151 | 104.981 | 58.916 | 16.457 | 1.00 | 32.03 | B | C |
| ATOM | 4771 | C | ILE | 151 | 102.978 | 58.008 | 21.016 | 1.00 | 33.74 | B | C |
| ATOM | 4772 | O | ILE | 151 | 103.593 | 57.013 | 21.394 | 1.00 | 33.98 | B | O |
| ATOM | 4773 | N | VAL | 152 | 101.725 | 58.254 | 21.368 | 1.00 | 29.85 | B | N |
| ATOM | 4774 | CA | VAL | 152 | 100.996 | 57.347 | 22.243 | 1.00 | 30.70 | B | C |
| ATOM | 4775 | CB | VAL | 152 | 100.279 | 58.127 | 23.344 | 1.00 | 30.57 | B | C |
| ATOM | 4776 | CG1 | VAL | 152 | 99.721 | 57.170 | 24.385 | 1.00 | 29.70 | B | C |
| ATOM | 4777 | CG2 | VAL | 152 | 101.245 | 59.134 | 23.962 | 1.00 | 27.01 | B | C |
| ATOM | 4778 | C | VAL | 152 | 99.966 | 56.560 | 21.451 | 1.00 | 28.60 | B | C |
| ATOM | 4779 | O | VAL | 152 | 98.867 | 57.044 | 21.194 | 1.00 | 22.20 | B | O |
| ATOM | 4780 | N | LEU | 153 | 100.324 | 55.336 | 21.083 | 1.00 | 26.94 | B | N |
| ATOM | 4781 | CA | LEU | 153 | 99.451 | 54.479 | 20.289 | 1.00 | 27.05 | B | C |
| ATOM | 4782 | CB | LEU | 153 | 100.312 | 53.600 | 19.370 | 1.00 | 31.93 | B | C |
| ATOM | 4783 | CG | LEU | 153 | 100.518 | 54.010 | 17.910 | 1.00 | 33.71 | B | C |
| ATOM | 4784 | CD1 | LEU | 153 | 100.287 | 55.490 | 17.732 | 1.00 | 34.22 | B | C |
| ATOM | 4785 | CD2 | LEU | 153 | 101.914 | 53.616 | 17.481 | 1.00 | 36.25 | B | C |
| ATOM | 4786 | C | LEU | 153 | 98.475 | 53.597 | 21.058 | 1.00 | 28.11 | B | C |
| ATOM | 4787 | O | LEU | 153 | 98.837 | 52.930 | 22.035 | 1.00 | 27.11 | B | O |
| ATOM | 4788 | N | ASP | 154 | 97.228 | 53.602 | 20.604 | 1.00 | 33.48 | B | N |
| ATOM | 4789 | CA | ASP | 154 | 96.199 | 52.768 | 21.204 | 1.00 | 32.96 | B | C |
| ATOM | 4790 | CB | ASP | 154 | 94.809 | 53.341 | 20.911 | 1.00 | 34.05 | B | C |
| ATOM | 4791 | CG | ASP | 154 | 93.886 | 52.502 | 21.505 | 1.00 | 33.25 | B | C |
| ATOM | 4792 | OD1 | ASP | 154 | 93.959 | 51.385 | 21.985 | 1.00 | 36.76 | B | O |
| ATOM | 4793 | OD2 | ASP | 154 | 92.523 | 52.960 | 21.489 | 1.00 | 29.57 | B | O |
| ATOM | 4794 | C | ASP | 154 | 96.362 | 51.412 | 20.515 | 1.00 | 36.30 | B | C |
| ATOM | 4795 | O | ASP | 154 | 96.349 | 51.326 | 19.285 | 1.00 | 32.62 | B | O |
| ATOM | 4796 | N | GLY | 155 | 96.539 | 50.361 | 21.303 | 1.00 | 16.68 | B | N |
| ATOM | 4797 | CA | GLY | 155 | 96.700 | 49.039 | 20.732 | 1.00 | 18.75 | B | C |
| ATOM | 4798 | C | GLY | 155 | 95.706 | 48.058 | 21.321 | 1.00 | 20.01 | B | C |
| ATOM | 4799 | O | GLY | 155 | 95.856 | 46.845 | 21.177 | 1.00 | 22.50 | B | O |
| ATOM | 4800 | N | SER | 156 | 94.692 | 48.595 | 21.992 | 1.00 | 30.46 | B | N |
| ATOM | 4801 | CA | SER | 156 | 93.653 | 47.780 | 22.612 | 1.00 | 35.04 | B | C |
| ATOM | 4802 | CB | SER | 156 | 92.616 | 48.670 | 23.302 | 1.00 | 22.70 | B | C |
| ATOM | 4803 | OG | SER | 156 | 91.999 | 49.542 | 22.372 | 1.00 | 25.62 | B | O |
| ATOM | 4804 | C | SER | 156 | 92.962 | 46.891 | 21.584 | 1.00 | 32.03 | B | C |
| ATOM | 4805 | O | SER | 156 | 93.057 | 47.122 | 20.379 | 1.00 | 35.21 | B | O |
| ATOM | 4806 | N | ASN | 157 | 92.257 | 45.879 | 22.074 | 1.00 | 34.08 | B | N |
| ATOM | 4807 | CA | ASN | 157 | 91.565 | 44.927 | 21.216 | 1.00 | 31.16 | B | C |
| ATOM | 4808 | CB | ASN | 157 | 90.632 | 44.046 | 22.047 | 1.00 | 34.61 | B | C |
| ATOM | 4809 | CG | ASN | 157 | 91.378 | 42.971 | 22.811 | 1.00 | 36.10 | B | C |
| ATOM | 4810 | OD1 | ASN | 157 | 90.795 | 42.270 | 23.638 | 1.00 | 33.17 | B | O |
| ATOM | 4811 | ND2 | ASN | 157 | 92.672 | 42.832 | 22.536 | 1.00 | 33.38 | B | N |
| ATOM | 4812 | C | ASN | 157 | 90.783 | 45.529 | 20.069 | 1.00 | 29.13 | B | C |
| ATOM | 4813 | O | ASN | 157 | 90.806 | 45.003 | 18.956 | 1.00 | 27.11 | B | O |
| ATOM | 4814 | N | SER | 158 | 90.094 | 46.631 | 20.339 | 1.00 | 20.01 | B | N |
| ATOM | 4815 | CA | SER | 158 | 89.275 | 47.285 | 19.324 | 1.00 | 18.22 | B | C |
| ATOM | 4816 | CB | SER | 158 | 88.506 | 48.464 | 19.936 | 1.00 | 15.08 | B | C |
| ATOM | 4817 | OG | SER | 158 | 89.356 | 49.363 | 20.616 | 1.00 | 17.79 | B | O |
| ATOM | 4818 | C | SER | 158 | 90.035 | 47.739 | 18.087 | 1.00 | 18.99 | B | C |

Fig. 19: A-67

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 4819 | O | SER | 158 | 89.527 | 47.602 | 16.984 | 1.00 | 16.16 | B | O |
| ATOM | 4820 | N | ILE | 159 | 91.245 | 48.269 | 18.257 | 1.00 | 19.55 | B | N |
| ATOM | 4821 | CA | ILE | 159 | 92.033 | 48.722 | 17.110 | 1.00 | 24.15 | B | C |
| ATOM | 4822 | CB | ILE | 159 | 93.423 | 49.203 | 17.541 | 1.00 | 21.45 | B | C |
| ATOM | 4823 | CG2 | ILE | 159 | 94.256 | 49.546 | 16.307 | 1.00 | 21.36 | B | C |
| ATOM | 4824 | CG1 | ILE | 159 | 93.293 | 50.411 | 18.471 | 1.00 | 26.23 | B | C |
| ATOM | 4825 | CD1 | ILE | 159 | 92.779 | 51.664 | 17.787 | 1.00 | 31.39 | B | C |
| ATOM | 4826 | C | ILE | 159 | 92.204 | 47.597 | 16.089 | 1.00 | 28.46 | B | C |
| ATOM | 4827 | O | ILE | 159 | 92.638 | 46.502 | 16.434 | 1.00 | 27.87 | B | O |
| ATOM | 4828 | N | TYR | 160 | 91.863 | 47.876 | 14.832 | 1.00 | 56.09 | B | N |
| ATOM | 4829 | CA | TYR | 160 | 91.959 | 46.886 | 13.756 | 1.00 | 58.22 | B | C |
| ATOM | 4830 | CB | TYR | 160 | 90.931 | 45.768 | 13.980 | 1.00 | 40.50 | B | C |
| ATOM | 4831 | CG | TYR | 160 | 90.932 | 44.654 | 12.939 | 1.00 | 37.26 | B | C |
| ATOM | 4832 | CD1 | TYR | 160 | 91.606 | 43.449 | 13.172 | 1.00 | 39.68 | B | C |
| ATOM | 4833 | CE1 | TYR | 160 | 91.602 | 42.423 | 12.225 | 1.00 | 37.28 | B | C |
| ATOM | 4834 | CD2 | TYR | 160 | 90.254 | 44.803 | 11.722 | 1.00 | 34.91 | B | C |
| ATOM | 4835 | CE2 | TYR | 160 | 90.251 | 43.782 | 10.770 | 1.00 | 38.62 | B | C |
| ATOM | 4836 | CZ | TYR | 160 | 90.926 | 42.598 | 11.030 | 1.00 | 37.97 | B | C |
| ATOM | 4837 | OH | TYR | 160 | 90.922 | 41.597 | 10.095 | 1.00 | 42.97 | B | O |
| ATOM | 4838 | C | TYR | 160 | 91.696 | 47.533 | 12.400 | 1.00 | 59.94 | B | C |
| ATOM | 4839 | O | TYR | 160 | 90.730 | 48.276 | 12.232 | 1.00 | 65.86 | B | O |
| ATOM | 4840 | N | PRO | 161 | 92.548 | 47.241 | 11.407 | 1.00 | 26.83 | B | N |
| ATOM | 4841 | CD | PRO | 161 | 92.182 | 47.499 | 10.002 | 1.00 | 24.03 | B | C |
| ATOM | 4842 | CA | PRO | 161 | 93.721 | 46.362 | 11.479 | 1.00 | 25.11 | B | C |
| ATOM | 4843 | CB | PRO | 161 | 93.784 | 45.785 | 10.075 | 1.00 | 28.41 | B | C |
| ATOM | 4844 | CG | PRO | 161 | 93.364 | 46.960 | 9.239 | 1.00 | 31.57 | B | C |
| ATOM | 4845 | C | PRO | 161 | 95.008 | 47.109 | 11.857 | 1.00 | 23.77 | B | C |
| ATOM | 4846 | O | PRO | 161 | 95.234 | 48.238 | 11.413 | 1.00 | 23.09 | B | O |
| ATOM | 4847 | N | TRP | 162 | 95.856 | 46.463 | 12.654 | 1.00 | 23.22 | B | N |
| ATOM | 4848 | CA | TRP | 162 | 97.108 | 47.062 | 13.111 | 1.00 | 24.29 | B | C |
| ATOM | 4849 | CB | TRP | 162 | 97.922 | 46.022 | 13.878 | 1.00 | 29.42 | B | C |
| ATOM | 4850 | CG | TRP | 162 | 99.067 | 46.586 | 14.670 | 1.00 | 29.94 | B | C |
| ATOM | 4851 | CD2 | TRP | 162 | 99.004 | 47.603 | 15.676 | 1.00 | 24.78 | B | C |
| ATOM | 4852 | CE2 | TRP | 162 | 100.308 | 47.769 | 16.185 | 1.00 | 28.33 | B | C |
| ATOM | 4853 | CE3 | TRP | 162 | 97.973 | 48.389 | 16.201 | 1.00 | 24.19 | B | C |
| ATOM | 4854 | CD1 | TRP | 162 | 100.369 | 46.192 | 14.611 | 1.00 | 29.13 | B | C |
| ATOM | 4855 | NE1 | TRP | 162 | 101.123 | 46.898 | 15.516 | 1.00 | 31.00 | B | N |
| ATOM | 4856 | CZ2 | TRP | 162 | 100.607 | 48.687 | 17.195 | 1.00 | 26.87 | B | C |
| ATOM | 4857 | CZ3 | TRP | 162 | 98.274 | 49.303 | 17.208 | 1.00 | 22.52 | B | C |
| ATOM | 4858 | CH2 | TRP | 162 | 99.580 | 49.441 | 17.691 | 1.00 | 27.43 | B | C |
| ATOM | 4859 | C | TRP | 162 | 97.961 | 47.663 | 11.988 | 1.00 | 26.07 | B | C |
| ATOM | 4860 | O | TRP | 162 | 98.554 | 48.734 | 12.161 | 1.00 | 25.22 | B | O |
| ATOM | 4861 | N | GLU | 163 | 98.010 | 46.979 | 10.843 | 1.00 | 39.64 | B | N |
| ATOM | 4862 | CA | GLU | 163 | 98.797 | 47.432 | 9.693 | 1.00 | 41.42 | B | C |
| ATOM | 4863 | CB | GLU | 163 | 98.585 | 46.509 | 8.485 | 1.00 | 121.98 | B | C |
| ATOM | 4864 | CG | GLU | 163 | 97.219 | 46.612 | 7.826 | 1.00 | 128.29 | B | C |
| ATOM | 4865 | CD | GLU | 163 | 97.206 | 46.043 | 6.418 | 1.00 | 130.43 | B | C |
| ATOM | 4866 | OE1 | GLU | 163 | 97.894 | 46.611 | 5.541 | 1.00 | 132.14 | B | O |
| ATOM | 4867 | OE2 | GLU | 163 | 96.512 | 45.029 | 6.187 | 1.00 | 129.39 | B | O |
| ATOM | 4868 | C | GLU | 163 | 98.491 | 48.867 | 9.280 | 1.00 | 41.08 | B | C |
| ATOM | 4869 | O | GLU | 163 | 99.390 | 49.609 | 8.881 | 1.00 | 37.25 | B | O |
| ATOM | 4870 | N | SER | 164 | 97.225 | 49.262 | 9.368 | 1.00 | 24.58 | B | N |
| ATOM | 4871 | CA | SER | 164 | 96.850 | 50.620 | 8.989 | 1.00 | 21.77 | B | C |
| ATOM | 4872 | CB | SER | 164 | 95.320 | 50.772 | 8.984 | 1.00 | 53.34 | B | C |
| ATOM | 4873 | OG | SER | 164 | 94.722 | 49.950 | 7.992 | 1.00 | 59.23 | B | O |
| ATOM | 4874 | C | SER | 164 | 97.484 | 51.619 | 9.956 | 1.00 | 22.53 | B | C |
| ATOM | 4875 | O | SER | 164 | 97.993 | 52.661 | 9.536 | 1.00 | 25.73 | B | O |
| ATOM | 4876 | N | VAL | 165 | 97.451 | 51.286 | 11.247 | 1.00 | 28.47 | B | N |
| ATOM | 4877 | CA | VAL | 165 | 98.027 | 52.137 | 12.280 | 1.00 | 27.86 | B | C |
| ATOM | 4878 | CB | VAL | 165 | 97.841 | 51.525 | 13.680 | 1.00 | 11.01 | B | C |
| ATOM | 4879 | CG1 | VAL | 165 | 98.722 | 52.245 | 14.697 | 1.00 | 12.40 | B | C |
| ATOM | 4880 | CG2 | VAL | 165 | 96.376 | 51.622 | 14.089 | 1.00 | 14.01 | B | C |
| ATOM | 4881 | C | VAL | 165 | 99.509 | 52.334 | 12.028 | 1.00 | 29.02 | B | C |
| ATOM | 4882 | O | VAL | 165 | 100.032 | 53.444 | 12.137 | 1.00 | 30.84 | B | O |
| ATOM | 4883 | N | ILE | 166 | 100.184 | 51.248 | 11.678 | 1.00 | 20.94 | B | N |
| ATOM | 4884 | CA | ILE | 166 | 101.613 | 51.305 | 11.400 | 1.00 | 20.26 | B | C |
| ATOM | 4885 | CB | ILE | 166 | 102.211 | 49.894 | 11.330 | 1.00 | 40.92 | B | C |
| ATOM | 4886 | CG2 | ILE | 166 | 103.697 | 49.962 | 10.986 | 1.00 | 40.13 | B | C |
| ATOM | 4887 | CG1 | ILE | 166 | 102.017 | 49.214 | 12.687 | 1.00 | 40.78 | B | C |
| ATOM | 4888 | CD1 | ILE | 166 | 102.580 | 47.823 | 12.762 | 1.00 | 37.18 | B | C |
| ATOM | 4889 | C | ILE | 166 | 101.920 | 52.073 | 10.121 | 1.00 | 19.71 | B | C |
| ATOM | 4890 | O | ILE | 166 | 102.909 | 52.792 | 10.059 | 1.00 | 21.46 | B | O |
| ATOM | 4891 | N | ALA | 167 | 101.076 | 51.927 | 9.106 | 1.00 | 22.08 | B | N |

Fig. 19: A-68

```
ATOM   4892  CA  ALA   167     101.271  52.670   7.866  1.00  22.68      B     C
ATOM   4893  CB  ALA   167     100.207  52.309   6.859  1.00   1.87      B     C
ATOM   4894  C   ALA   167     101.165  54.150   8.224  1.00  23.89      B     C
ATOM   4895  O   ALA   167     101.881  54.989   7.684  1.00  20.49      B     O
ATOM   4896  N   PHE   168     100.261  54.458   9.147  1.00  25.99      B     N
ATOM   4897  CA  PHE   168     100.083  55.823   9.583  1.00  24.51      B     C
ATOM   4898  CB  PHE   168      98.964  55.902  10.623  1.00  28.51      B     C
ATOM   4899  CG  PHE   168      98.962  57.185  11.406  1.00  27.01      B     C
ATOM   4900  CD1 PHE   168      99.549  57.240  12.671  1.00  28.61      B     C
ATOM   4901  CD2 PHE   168      98.409  58.341  10.872  1.00  25.32      B     C
ATOM   4902  CE1 PHE   168      99.587  58.424  13.392  1.00  27.09      B     C
ATOM   4903  CE2 PHE   168      98.442  59.529  11.587  1.00  27.14      B     C
ATOM   4904  CZ  PHE   168      99.034  59.570  12.853  1.00  29.63      B     C
ATOM   4905  C   PHE   168     101.397  56.325  10.178  1.00  25.37      B     C
ATOM   4906  O   PHE   168     101.832  57.446   9.908  1.00  21.81      B     O
ATOM   4907  N   LEU   169     102.030  55.488  10.990  1.00  25.37      B     N
ATOM   4908  CA  LEU   169     103.286  55.867  11.611  1.00  27.96      B     C
ATOM   4909  CB  LEU   169     103.749  54.790  12.585  1.00  24.35      B     C
ATOM   4910  CG  LEU   169     103.127  54.723  13.977  1.00  23.51      B     C
ATOM   4911  CD1 LEU   169     103.983  53.810  14.831  1.00  19.97      B     C
ATOM   4912  CD2 LEU   169     103.079  56.105  14.609  1.00  20.37      B     C
ATOM   4913  C   LEU   169     104.357  56.081  10.555  1.00  30.26      B     C
ATOM   4914  O   LEU   169     105.055  57.095  10.555  1.00  31.69      B     O
ATOM   4915  N   ASN   170     104.488  55.115   9.655  1.00  28.40      B     N
ATOM   4916  CA  ASN   170     105.470  55.208   8.591  1.00  25.53      B     C
ATOM   4917  CB  ASN   170     105.243  54.077   7.580  1.00  72.75      B     C
ATOM   4918  CG  ASN   170     106.484  53.768   6.747  1.00  76.17      B     C
ATOM   4919  OD1 ASN   170     106.703  54.346   5.680  1.00  71.70      B     O
ATOM   4920  ND2 ASN   170     107.307  52.854   7.242  1.00  74.08      B     N
ATOM   4921  C   ASN   170     105.335  56.578   7.913  1.00  25.54      B     C
ATOM   4922  O   ASN   170     106.242  57.408   7.992  1.00  25.75      B     O
ATOM   4923  N   ASP   171     104.189  56.819   7.275  1.00  35.44      B     N
ATOM   4924  CA  ASP   171     103.940  58.079   6.581  1.00  37.56      B     C
ATOM   4925  CB  ASP   171     102.467  58.179   6.168  1.00  72.00      B     C
ATOM   4926  CG  ASP   171     102.163  57.427   4.880  1.00  79.65      B     C
ATOM   4927  OD1 ASP   171     102.448  56.213   4.805  1.00  81.87      B     O
ATOM   4928  OD2 ASP   171     101.635  58.055   3.937  1.00  81.51      B     O
ATOM   4929  C   ASP   171     104.309  59.289   7.418  1.00  39.05      B     C
ATOM   4930  O   ASP   171     104.975  60.202   6.937  1.00  37.77      B     O
ATOM   4931  N   LEU   172     103.881  59.289   8.674  1.00  36.54      B     N
ATOM   4932  CA  LEU   172     104.152  60.403   9.570  1.00  37.22      B     C
ATOM   4933  CB  LEU   172     103.410  60.204  10.891  1.00  36.27      B     C
ATOM   4934  CG  LEU   172     102.901  61.423  11.674  1.00  35.76      B     C
ATOM   4935  CD1 LEU   172     103.145  61.178  13.158  1.00  33.36      B     C
ATOM   4936  CD2 LEU   172     103.593  62.706  11.237  1.00  33.93      B     C
ATOM   4937  C   LEU   172     105.642  60.561   9.849  1.00  37.56      B     C
ATOM   4938  O   LEU   172     106.212  61.628   9.627  1.00  37.55      B     O
ATOM   4939  N   LEU   173     106.269  59.493  10.337  1.00  40.49      B     N
ATOM   4940  CA  LEU   173     107.692  59.520  10.669  1.00  43.24      B     C
ATOM   4941  CB  LEU   173     108.115  58.215  11.364  1.00  18.13      B     C
ATOM   4942  CG  LEU   173     107.801  57.866  12.826  1.00  19.48      B     C
ATOM   4943  CD1 LEU   173     108.033  59.060  13.729  1.00  23.00      B     C
ATOM   4944  CD2 LEU   173     106.380  57.395  12.943  1.00  20.03      B     C
ATOM   4945  C   LEU   173     108.650  59.772   9.503  1.00  44.67      B     C
ATOM   4946  O   LEU   173     109.601  60.537   9.642  1.00  41.39      B     O
ATOM   4947  N   LYS   174     108.409  59.135   8.360  1.00  37.56      B     N
ATOM   4948  CA  LYS   174     109.304  59.291   7.221  1.00  37.78      B     C
ATOM   4949  CB  LYS   174     108.836  58.421   6.047  1.00  42.14      B     C
ATOM   4950  CG  LYS   174     107.739  58.988   5.169  1.00  42.47      B     C
ATOM   4951  CD  LYS   174     107.472  58.022   4.008  1.00  41.72      B     C
ATOM   4952  CE  LYS   174     106.689  58.660   2.852  1.00  36.97      B     C
ATOM   4953  NZ  LYS   174     105.297  59.097   3.187  1.00  33.44      B     N
ATOM   4954  C   LYS   174     109.511  60.738   6.774  1.00  36.14      B     C
ATOM   4955  O   LYS   174     110.571  61.078   6.245  1.00  37.01      B     O
ATOM   4956  N   ARG   175     108.514  61.589   7.004  1.00  41.42      B     N
ATOM   4957  CA  ARG   175     108.587  63.006   6.635  1.00  43.65      B     C
ATOM   4958  CB  ARG   175     107.182  63.634   6.654  1.00 108.28      B     C
ATOM   4959  CG  ARG   175     106.189  63.149   5.589  1.00 115.21      B     C
ATOM   4960  CD  ARG   175     104.762  63.613   5.939  1.00 119.49      B     C
ATOM   4961  NE  ARG   175     103.895  63.818   4.775  1.00 124.39      B     N
ATOM   4962  CZ  ARG   175     103.454  62.856   3.969  1.00 127.97      B     C
ATOM   4963  NH1 ARG   175     103.793  61.593   4.182  1.00 128.17      B     N
ATOM   4964  NH2 ARG   175     102.666  63.162   2.945  1.00 128.87      B     N
```

Fig. 19: A-69

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 4965 | C | ARG | 175 | 109.471 | 63.798 | 7.611 | 1.00 | 41.18 | B | C |
| ATOM | 4966 | O | ARG | 175 | 109.696 | 64.986 | 7.411 | 1.00 | 41.02 | B | O |
| ATOM | 4967 | N | MET | 176 | 109.970 | 63.145 | 8.660 | 1.00 | 47.15 | B | N |
| ATOM | 4968 | CA | MET | 176 | 110.777 | 63.821 | 9.678 | 1.00 | 43.63 | B | C |
| ATOM | 4969 | CB | MET | 176 | 110.320 | 63.383 | 11.065 | 1.00 | 33.29 | B | C |
| ATOM | 4970 | CG | MET | 176 | 108.969 | 63.920 | 11.456 | 1.00 | 30.19 | B | C |
| ATOM | 4971 | SD | MET | 176 | 108.444 | 63.366 | 13.073 | 1.00 | 34.33 | B | S |
| ATOM | 4972 | CE | MET | 176 | 107.041 | 62.339 | 12.619 | 1.00 | 27.84 | B | C |
| ATOM | 4973 | C | MET | 176 | 112.284 | 63.663 | 9.611 | 1.00 | 47.14 | B | C |
| ATOM | 4974 | O | MET | 176 | 112.795 | 62.707 | 9.037 | 1.00 | 47.21 | B | O |
| ATOM | 4975 | N | ASP | 177 | 112.991 | 64.617 | 10.213 | 1.00 | 51.06 | B | N |
| ATOM | 4976 | CA | ASP | 177 | 114.451 | 64.590 | 10.276 | 1.00 | 53.55 | B | C |
| ATOM | 4977 | CB | ASP | 177 | 115.047 | 65.944 | 9.881 | 1.00 | 101.95 | B | C |
| ATOM | 4978 | CG | ASP | 177 | 115.065 | 66.158 | 8.381 | 1.00 | 104.90 | B | C |
| ATOM | 4979 | OD1 | ASP | 177 | 115.635 | 67.174 | 7.934 | 1.00 | 104.57 | B | O |
| ATOM | 4980 | OD2 | ASP | 177 | 114.511 | 65.310 | 7.647 | 1.00 | 106.55 | B | O |
| ATOM | 4981 | C | ASP | 177 | 114.851 | 64.249 | 11.706 | 1.00 | 53.47 | B | C |
| ATOM | 4982 | O | ASP | 177 | 115.107 | 65.133 | 12.519 | 1.00 | 53.19 | B | O |
| ATOM | 4983 | N | ILE | 178 | 114.888 | 62.954 | 12.003 | 1.00 | 55.91 | B | N |
| ATOM | 4984 | CA | ILE | 178 | 115.236 | 62.465 | 13.331 | 1.00 | 56.05 | B | C |
| ATOM | 4985 | CB | ILE | 178 | 114.719 | 61.004 | 13.543 | 1.00 | 33.37 | B | C |
| ATOM | 4986 | CG2 | ILE | 178 | 115.323 | 60.410 | 14.790 | 1.00 | 31.65 | B | C |
| ATOM | 4987 | CG1 | ILE | 178 | 113.191 | 60.985 | 13.665 | 1.00 | 34.43 | B | C |
| ATOM | 4988 | CD1 | ILE | 178 | 112.464 | 60.671 | 12.376 | 1.00 | 36.27 | B | C |
| ATOM | 4989 | C | ILE | 178 | 116.743 | 62.502 | 13.583 | 1.00 | 55.19 | B | C |
| ATOM | 4990 | O | ILE | 178 | 117.543 | 62.224 | 12.686 | 1.00 | 57.18 | B | O |
| ATOM | 4991 | N | GLY | 179 | 117.117 | 62.846 | 14.812 | 1.00 | 23.09 | B | N |
| ATOM | 4992 | CA | GLY | 179 | 118.521 | 62.912 | 15.178 | 1.00 | 22.81 | B | C |
| ATOM | 4993 | C | GLY | 179 | 118.736 | 63.508 | 16.560 | 1.00 | 23.57 | B | C |
| ATOM | 4994 | O | GLY | 179 | 117.931 | 64.325 | 17.012 | 1.00 | 21.72 | B | O |
| ATOM | 4995 | N | PRO | 180 | 119.815 | 63.113 | 17.265 | 1.00 | 39.73 | B | N |
| ATOM | 4996 | CD | PRO | 180 | 120.782 | 62.068 | 16.873 | 1.00 | 73.51 | B | C |
| ATOM | 4997 | CA | PRO | 180 | 120.124 | 63.620 | 18.606 | 1.00 | 40.79 | B | C |
| ATOM | 4998 | CB | PRO | 180 | 121.542 | 63.113 | 18.840 | 1.00 | 72.35 | B | C |
| ATOM | 4999 | CG | PRO | 180 | 121.502 | 61.776 | 18.184 | 1.00 | 74.74 | B | C |
| ATOM | 5000 | C | PRO | 180 | 120.019 | 65.135 | 18.697 | 1.00 | 42.57 | B | C |
| ATOM | 5001 | O | PRO | 180 | 119.718 | 65.680 | 19.761 | 1.00 | 43.21 | B | O |
| ATOM | 5002 | N | LYS | 181 | 120.268 | 65.810 | 17.578 | 1.00 | 56.97 | B | N |
| ATOM | 5003 | CA | LYS | 181 | 120.186 | 67.265 | 17.534 | 1.00 | 57.39 | B | C |
| ATOM | 5004 | CB | LYS | 181 | 121.522 | 67.867 | 17.092 | 1.00 | 83.43 | B | C |
| ATOM | 5005 | CG | LYS | 181 | 122.677 | 67.613 | 18.052 | 1.00 | 84.03 | B | C |
| ATOM | 5006 | CD | LYS | 181 | 122.430 | 68.205 | 19.442 | 1.00 | 82.89 | B | C |
| ATOM | 5007 | CE | LYS | 181 | 123.580 | 67.868 | 20.394 | 1.00 | 85.41 | B | C |
| ATOM | 5008 | NZ | LYS | 181 | 123.351 | 68.348 | 21.790 | 1.00 | 84.98 | B | N |
| ATOM | 5009 | C | LYS | 181 | 119.070 | 67.736 | 16.597 | 1.00 | 56.74 | B | C |
| ATOM | 5010 | O | LYS | 181 | 118.973 | 68.917 | 16.274 | 1.00 | 55.06 | B | O |
| ATOM | 5011 | N | GLN | 182 | 118.225 | 66.804 | 16.167 | 1.00 | 33.36 | B | N |
| ATOM | 5012 | CA | GLN | 182 | 117.112 | 67.117 | 15.279 | 1.00 | 32.02 | B | C |
| ATOM | 5013 | CB | GLN | 182 | 117.152 | 66.219 | 14.044 | 1.00 | 74.94 | B | C |
| ATOM | 5014 | CG | GLN | 182 | 118.512 | 66.050 | 13.424 | 1.00 | 76.22 | B | C |
| ATOM | 5015 | CD | GLN | 182 | 119.037 | 67.334 | 12.850 | 1.00 | 77.84 | B | C |
| ATOM | 5016 | OE1 | GLN | 182 | 119.266 | 68.305 | 13.573 | 1.00 | 78.68 | B | O |
| ATOM | 5017 | NE2 | GLN | 182 | 119.230 | 67.356 | 11.537 | 1.00 | 79.20 | B | N |
| ATOM | 5018 | C | GLN | 182 | 115.831 | 66.826 | 16.046 | 1.00 | 30.93 | B | C |
| ATOM | 5019 | O | GLN | 182 | 115.638 | 67.278 | 17.173 | 1.00 | 35.26 | B | O |
| ATOM | 5020 | N | THR | 183 | 114.961 | 66.046 | 15.419 | 1.00 | 29.87 | B | N |
| ATOM | 5021 | CA | THR | 183 | 113.706 | 65.648 | 16.025 | 1.00 | 26.79 | B | C |
| ATOM | 5022 | CB | THR | 183 | 112.612 | 65.493 | 14.962 | 1.00 | 31.40 | B | C |
| ATOM | 5023 | OG1 | THR | 183 | 112.484 | 66.721 | 14.231 | 1.00 | 27.85 | B | O |
| ATOM | 5024 | CG2 | THR | 183 | 111.285 | 65.127 | 15.610 | 1.00 | 29.08 | B | C |
| ATOM | 5025 | C | THR | 183 | 113.957 | 64.288 | 16.666 | 1.00 | 26.45 | B | C |
| ATOM | 5026 | O | THR | 183 | 114.624 | 63.428 | 16.077 | 1.00 | 24.98 | B | O |
| ATOM | 5027 | N | GLN | 184 | 113.464 | 64.102 | 17.883 | 1.00 | 44.27 | B | N |
| ATOM | 5028 | CA | GLN | 184 | 113.619 | 62.822 | 18.546 | 1.00 | 39.92 | B | C |
| ATOM | 5029 | CB | GLN | 184 | 114.254 | 62.981 | 19.920 | 1.00 | 33.99 | B | C |
| ATOM | 5030 | CG | GLN | 184 | 115.752 | 63.197 | 19.878 | 1.00 | 33.74 | B | C |
| ATOM | 5031 | CD | GLN | 184 | 116.427 | 62.766 | 21.163 | 1.00 | 33.21 | B | C |
| ATOM | 5032 | OE1 | GLN | 184 | 116.097 | 63.258 | 22.244 | 1.00 | 28.91 | B | O |
| ATOM | 5033 | NE2 | GLN | 184 | 117.375 | 61.835 | 21.053 | 1.00 | 31.51 | B | N |
| ATOM | 5034 | C | GLN | 184 | 112.227 | 62.240 | 18.670 | 1.00 | 40.30 | B | C |
| ATOM | 5035 | O | GLN | 184 | 111.249 | 62.978 | 18.834 | 1.00 | 37.69 | B | O |
| ATOM | 5036 | N | VAL | 185 | 112.131 | 60.918 | 18.574 | 1.00 | 24.17 | B | N |
| ATOM | 5037 | CA | VAL | 185 | 110.837 | 60.255 | 18.649 | 1.00 | 22.54 | B | C |

Fig. 19: A-70

```
ATOM   5038  CB  VAL   185     110.345  59.858  17.235  1.00  12.44      B    C
ATOM   5039  CG1 VAL   185     109.105  58.990  17.335  1.00  12.43      B    C
ATOM   5040  CG2 VAL   185     110.052  61.103  16.425  1.00   1.87      B    C
ATOM   5041  C   VAL   185     110.840  59.025  19.536  1.00  23.13      B    C
ATOM   5042  O   VAL   185     111.756  58.206  19.510  1.00  20.28      B    O
ATOM   5043  N   GLY   186     109.789  58.914  20.328  1.00  27.91      B    N
ATOM   5044  CA  GLY   186     109.630  57.782  21.213  1.00  29.54      B    C
ATOM   5045  C   GLY   186     108.200  57.319  21.045  1.00  27.52      B    C
ATOM   5046  O   GLY   186     107.308  58.138  20.839  1.00  32.88      B    O
ATOM   5047  N   ILE   187     107.970  56.017  21.105  1.00  20.77      B    N
ATOM   5048  CA  ILE   187     106.617  55.519  20.958  1.00  19.36      B    C
ATOM   5049  CB  ILE   187     106.460  54.729  19.642  1.00  17.70      B    C
ATOM   5050  CG2 ILE   187     105.081  54.079  19.577  1.00  15.03      B    C
ATOM   5051  CG1 ILE   187     106.639  55.676  18.454  1.00  18.22      B    C
ATOM   5052  CD1 ILE   187     106.437  55.033  17.100  1.00  19.27      B    C
ATOM   5053  C   ILE   187     106.160  54.674  22.143  1.00  18.65      B    C
ATOM   5054  O   ILE   187     106.852  53.763  22.590  1.00  17.55      B    O
ATOM   5055  N   VAL   188     104.984  55.015  22.649  1.00  23.72      B    N
ATOM   5056  CA  VAL   188     104.370  54.332  23.774  1.00  23.39      B    C
ATOM   5057  CB  VAL   188     104.053  55.333  24.911  1.00  24.28      B    C
ATOM   5058  CG1 VAL   188     103.055  54.728  25.896  1.00  19.55      B    C
ATOM   5059  CG2 VAL   188     105.320  55.715  25.625  1.00  24.70      B    C
ATOM   5060  C   VAL   188     103.055  53.702  23.303  1.00  21.93      B    C
ATOM   5061  O   VAL   188     102.274  54.341  22.591  1.00  21.34      B    O
ATOM   5062  N   GLN   189     102.815  52.453  23.686  1.00  21.90      B    N
ATOM   5063  CA  GLN   189     101.580  51.785  23.312  1.00  21.58      B    C
ATOM   5064  CB  GLN   189     101.857  50.545  22.463  1.00  19.75      B    C
ATOM   5065  CG  GLN   189     100.577  49.784  22.128  1.00  17.26      B    C
ATOM   5066  CD  GLN   189     100.819  48.495  21.377  1.00  17.97      B    C
ATOM   5067  OE1 GLN   189      99.930  47.647  21.283  1.00  19.19      B    O
ATOM   5068  NE2 GLN   189     102.022  48.340  20.831  1.00  19.01      B    N
ATOM   5069  C   GLN   189     100.820  51.386  24.572  1.00  18.57      B    C
ATOM   5070  O   GLN   189     101.423  50.980  25.567  1.00  16.93      B    O
ATOM   5071  N   TYR   190      99.494  51.500  24.524  1.00  20.56      B    N
ATOM   5072  CA  TYR   190      98.671  51.159  25.680  1.00  24.08      B    C
ATOM   5073  CB  TYR   190      98.255  52.432  26.418  1.00  22.72      B    C
ATOM   5074  CG  TYR   190      97.213  53.255  25.687  1.00  17.37      B    C
ATOM   5075  CD1 TYR   190      95.849  53.072  25.929  1.00  15.48      B    C
ATOM   5076  CE1 TYR   190      94.882  53.820  25.244  1.00  17.37      B    C
ATOM   5077  CD2 TYR   190      97.586  54.207  24.739  1.00  13.48      B    C
ATOM   5078  CE2 TYR   190      96.624  54.957  24.051  1.00  14.90      B    C
ATOM   5079  CZ  TYR   190      95.279  54.760  24.311  1.00  15.79      B    C
ATOM   5080  OH  TYR   190      94.340  55.527  23.663  1.00  14.38      B    O
ATOM   5081  C   TYR   190      97.428  50.342  25.344  1.00  25.93      B    C
ATOM   5082  O   TYR   190      97.000  50.260  24.195  1.00  26.01      B    O
ATOM   5083  N   GLY   191      96.860  49.746  26.385  1.00  24.69      B    N
ATOM   5084  CA  GLY   191      95.675  48.920  26.270  1.00  22.44      B    C
ATOM   5085  C   GLY   191      95.277  48.649  27.701  1.00  23.88      B    C
ATOM   5086  O   GLY   191      94.720  49.532  28.348  1.00  27.26      B    O
ATOM   5087  N   GLU   192      95.572  47.446  28.197  1.00  23.59      B    N
ATOM   5088  CA  GLU   192      95.284  47.084  29.584  1.00  25.60      B    C
ATOM   5089  CB  GLU   192      95.232  45.574  29.758  1.00  40.14      B    C
ATOM   5090  CG  GLU   192      94.135  44.871  29.002  1.00  40.52      B    C
ATOM   5091  CD  GLU   192      94.134  43.382  29.273  1.00  40.71      B    C
ATOM   5092  OE1 GLU   192      93.230  42.690  28.759  1.00  43.60      B    O
ATOM   5093  OE2 GLU   192      95.038  42.906  29.999  1.00  38.58      B    O
ATOM   5094  C   GLU   192      96.465  47.608  30.390  1.00  25.41      B    C
ATOM   5095  O   GLU   192      96.325  48.027  31.536  1.00  26.78      B    O
ATOM   5096  N   ASN   193      97.637  47.569  29.770  1.00  17.36      B    N
ATOM   5097  CA  ASN   193      98.862  48.041  30.395  1.00  18.57      B    C
ATOM   5098  CB  ASN   193      99.814  46.877  30.653  1.00  57.60      B    C
ATOM   5099  CG  ASN   193      99.159  45.755  31.418  1.00  60.77      B    C
ATOM   5100  OD1 ASN   193      98.225  45.115  30.933  1.00  64.88      B    O
ATOM   5101  ND2 ASN   193      99.644  45.509  32.626  1.00  62.88      B    N
ATOM   5102  C   ASN   193      99.510  49.007  29.425  1.00  16.75      B    C
ATOM   5103  O   ASN   193      98.917  49.360  28.413  1.00  17.75      B    O
ATOM   5104  N   VAL   194     100.735  49.418  29.728  1.00  23.63      B    N
ATOM   5105  CA  VAL   194     101.454  50.346  28.866  1.00  25.97      B    C
ATOM   5106  CB  VAL   194     101.516  51.750  29.490  1.00  24.85      B    C
ATOM   5107  CG1 VAL   194     102.014  52.745  28.459  1.00  25.88      B    C
ATOM   5108  CG2 VAL   194     100.153  52.147  30.032  1.00  22.12      B    C
ATOM   5109  C   VAL   194     102.887  49.864  28.661  1.00  23.74      B    C
ATOM   5110  O   VAL   194     103.535  49.384  29.597  1.00  21.86      B    O
```

Fig. 19: A-71

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 5111 | N | THR | 195 | 103.397 | 49.986 | 27.444 | 1.00 | 25.03 | B | N |
| ATOM | 5112 | CA | THR | 195 | 104.758 | 49.552 | 27.197 | 1.00 | 26.21 | B | C |
| ATOM | 5113 | CB | THR | 195 | 104.797 | 48.182 | 26.450 | 1.00 | 38.61 | B | C |
| ATOM | 5114 | OG1 | THR | 195 | 104.420 | 48.360 | 25.081 | 1.00 | 42.62 | B | O |
| ATOM | 5115 | CG2 | THR | 195 | 103.828 | 47.195 | 27.087 | 1.00 | 40.24 | B | C |
| ATOM | 5116 | C | THR | 195 | 105.511 | 50.599 | 26.391 | 1.00 | 27.05 | B | C |
| ATOM | 5117 | O | THR | 195 | 104.944 | 51.254 | 25.514 | 1.00 | 29.64 | B | O |
| ATOM | 5118 | N | HIS | 196 | 106.791 | 50.765 | 26.716 | 1.00 | 33.64 | B | N |
| ATOM | 5119 | CA | HIS | 196 | 107.656 | 51.713 | 26.029 | 1.00 | 33.74 | B | C |
| ATOM | 5120 | CB | HIS | 196 | 108.815 | 52.119 | 26.942 | 1.00 | 34.91 | B | C |
| ATOM | 5121 | CG | HIS | 196 | 108.417 | 53.011 | 28.079 | 1.00 | 31.41 | B | C |
| ATOM | 5122 | CD2 | HIS | 196 | 108.084 | 52.725 | 29.360 | 1.00 | 32.04 | B | C |
| ATOM | 5123 | ND1 | HIS | 196 | 108.322 | 54.382 | 27.955 | 1.00 | 30.06 | B | N |
| ATOM | 5124 | CE1 | HIS | 196 | 107.949 | 54.901 | 29.111 | 1.00 | 26.78 | B | C |
| ATOM | 5125 | NE2 | HIS | 196 | 107.797 | 53.918 | 29.979 | 1.00 | 24.99 | B | N |
| ATOM | 5126 | C | HIS | 196 | 108.219 | 51.017 | 24.806 | 1.00 | 33.60 | B | C |
| ATOM | 5127 | O | HIS | 196 | 109.201 | 50.289 | 24.932 | 1.00 | 32.26 | B | O |
| ATOM | 5128 | N | GLU | 197 | 107.609 | 51.216 | 23.636 | 1.00 | 34.73 | B | N |
| ATOM | 5129 | CA | GLU | 197 | 108.123 | 50.583 | 22.417 | 1.00 | 32.06 | B | C |
| ATOM | 5130 | CB | GLU | 197 | 107.313 | 50.999 | 21.193 | 1.00 | 45.57 | B | C |
| ATOM | 5131 | CG | GLU | 197 | 105.913 | 50.386 | 21.130 | 1.00 | 45.91 | B | C |
| ATOM | 5132 | CD | GLU | 197 | 105.911 | 48.876 | 21.303 | 1.00 | 44.98 | B | C |
| ATOM | 5133 | OE1 | GLU | 197 | 106.869 | 48.228 | 20.834 | 1.00 | 43.56 | B | O |
| ATOM | 5134 | OE2 | GLU | 197 | 104.949 | 48.331 | 21.892 | 1.00 | 46.64 | B | O |
| ATOM | 5135 | C | GLU | 197 | 109.595 | 50.958 | 22.245 | 1.00 | 29.53 | B | C |
| ATOM | 5136 | O | GLU | 197 | 110.447 | 50.081 | 22.151 | 1.00 | 34.73 | B | O |
| ATOM | 5137 | N | PHE | 198 | 109.898 | 52.254 | 22.203 | 1.00 | 32.40 | B | N |
| ATOM | 5138 | CA | PHE | 198 | 111.293 | 52.691 | 22.126 | 1.00 | 34.20 | B | C |
| ATOM | 5139 | CB | PHE | 198 | 111.881 | 52.501 | 20.714 | 1.00 | 23.77 | B | C |
| ATOM | 5140 | CG | PHE | 198 | 111.239 | 53.331 | 19.636 | 1.00 | 22.02 | B | C |
| ATOM | 5141 | CD1 | PHE | 198 | 111.379 | 54.711 | 19.614 | 1.00 | 28.16 | B | C |
| ATOM | 5142 | CD2 | PHE | 198 | 110.539 | 52.715 | 18.597 | 1.00 | 16.76 | B | C |
| ATOM | 5143 | CE1 | PHE | 198 | 110.837 | 55.468 | 18.571 | 1.00 | 24.19 | B | C |
| ATOM | 5144 | CE2 | PHE | 198 | 109.990 | 53.460 | 17.548 | 1.00 | 22.67 | B | C |
| ATOM | 5145 | CZ | PHE | 198 | 110.140 | 54.838 | 17.536 | 1.00 | 26.47 | B | C |
| ATOM | 5146 | C | PHE | 198 | 111.471 | 54.120 | 22.642 | 1.00 | 36.88 | B | C |
| ATOM | 5147 | O | PHE | 198 | 110.631 | 54.973 | 22.398 | 1.00 | 38.17 | B | O |
| ATOM | 5148 | N | ASN | 199 | 112.552 | 54.366 | 23.386 | 1.00 | 21.75 | B | N |
| ATOM | 5149 | CA | ASN | 199 | 112.810 | 55.686 | 23.971 | 1.00 | 22.04 | B | C |
| ATOM | 5150 | CB | ASN | 199 | 113.924 | 55.613 | 25.007 | 1.00 | 33.57 | B | C |
| ATOM | 5151 | CG | ASN | 199 | 113.636 | 54.633 | 26.105 | 1.00 | 34.83 | B | C |
| ATOM | 5152 | OD1 | ASN | 199 | 112.614 | 54.717 | 26.785 | 1.00 | 36.36 | B | O |
| ATOM | 5153 | ND2 | ASN | 199 | 114.549 | 53.688 | 26.295 | 1.00 | 33.71 | B | N |
| ATOM | 5154 | C | ASN | 199 | 113.159 | 56.792 | 22.996 | 1.00 | 24.50 | B | C |
| ATOM | 5155 | O | ASN | 199 | 113.569 | 56.546 | 21.862 | 1.00 | 22.31 | B | O |
| ATOM | 5156 | N | LEU | 200 | 113.004 | 58.023 | 23.473 | 1.00 | 27.41 | B | N |
| ATOM | 5157 | CA | LEU | 200 | 113.286 | 59.215 | 22.685 | 1.00 | 29.37 | B | C |
| ATOM | 5158 | CB | LEU | 200 | 113.094 | 60.467 | 23.542 | 1.00 | 22.93 | B | C |
| ATOM | 5159 | CG | LEU | 200 | 111.694 | 61.088 | 23.545 | 1.00 | 20.78 | B | C |
| ATOM | 5160 | CD1 | LEU | 200 | 111.613 | 62.208 | 24.578 | 1.00 | 25.90 | B | C |
| ATOM | 5161 | CD2 | LEU | 200 | 111.375 | 61.607 | 22.140 | 1.00 | 21.95 | B | C |
| ATOM | 5162 | C | LEU | 200 | 114.685 | 59.223 | 22.104 | 1.00 | 29.77 | B | C |
| ATOM | 5163 | O | LEU | 200 | 114.899 | 59.698 | 20.992 | 1.00 | 30.79 | B | O |
| ATOM | 5164 | N | ASN | 201 | 115.635 | 58.685 | 22.856 | 1.00 | 32.06 | B | N |
| ATOM | 5165 | CA | ASN | 201 | 117.027 | 58.660 | 22.426 | 1.00 | 33.91 | B | C |
| ATOM | 5166 | CB | ASN | 201 | 117.920 | 59.105 | 23.578 | 1.00 | 34.75 | B | C |
| ATOM | 5167 | CG | ASN | 201 | 117.838 | 58.168 | 24.769 | 1.00 | 37.03 | B | C |
| ATOM | 5168 | OD1 | ASN | 201 | 118.389 | 58.443 | 25.832 | 1.00 | 37.17 | B | O |
| ATOM | 5169 | ND2 | ASN | 201 | 117.147 | 57.052 | 24.592 | 1.00 | 34.87 | B | N |
| ATOM | 5170 | C | ASN | 201 | 117.517 | 57.309 | 21.936 | 1.00 | 33.96 | B | C |
| ATOM | 5171 | O | ASN | 201 | 118.723 | 57.111 | 21.825 | 1.00 | 29.86 | B | O |
| ATOM | 5172 | N | LYS | 202 | 116.603 | 56.382 | 21.653 | 1.00 | 35.80 | B | N |
| ATOM | 5173 | CA | LYS | 202 | 116.990 | 55.051 | 21.183 | 1.00 | 35.92 | B | C |
| ATOM | 5174 | CB | LYS | 202 | 115.786 | 54.107 | 21.160 | 1.00 | 34.30 | B | C |
| ATOM | 5175 | CG | LYS | 202 | 116.107 | 52.652 | 20.788 | 1.00 | 35.84 | B | C |
| ATOM | 5176 | CD | LYS | 202 | 116.841 | 51.929 | 21.898 | 1.00 | 37.75 | B | C |
| ATOM | 5177 | CE | LYS | 202 | 116.185 | 52.179 | 23.273 | 1.00 | 43.50 | B | C |
| ATOM | 5178 | NZ | LYS | 202 | 114.729 | 51.801 | 23.388 | 1.00 | 42.52 | B | N |
| ATOM | 5179 | C | LYS | 202 | 117.617 | 55.071 | 19.800 | 1.00 | 34.79 | B | C |
| ATOM | 5180 | O | LYS | 202 | 118.667 | 54.472 | 19.589 | 1.00 | 32.07 | B | O |
| ATOM | 5181 | N | TYR | 203 | 116.977 | 55.747 | 18.852 | 1.00 | 23.81 | B | N |
| ATOM | 5182 | CA | TYR | 203 | 117.509 | 55.815 | 17.491 | 1.00 | 23.49 | B | C |
| ATOM | 5183 | CB | TYR | 203 | 116.466 | 55.300 | 16.499 | 1.00 | 32.41 | B | C |

Fig. 19: A-72

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 5184 | CG | TYR | 203 | 115.907 | 53.951 | 16.886 | 1.00 | 31.08 | B | C |
| ATOM | 5185 | CD1 | TYR | 203 | 114.665 | 53.844 | 17.509 | 1.00 | 31.69 | B | C |
| ATOM | 5186 | CE1 | TYR | 203 | 114.179 | 52.613 | 17.930 | 1.00 | 28.16 | B | C |
| ATOM | 5187 | CD2 | TYR | 203 | 116.649 | 52.784 | 16.689 | 1.00 | 33.97 | B | C |
| ATOM | 5188 | CE2 | TYR | 203 | 116.173 | 51.550 | 17.109 | 1.00 | 36.72 | B | C |
| ATOM | 5189 | CZ | TYR | 203 | 114.940 | 51.474 | 17.730 | 1.00 | 36.34 | B | C |
| ATOM | 5190 | OH | TYR | 203 | 114.466 | 50.262 | 18.169 | 1.00 | 41.34 | B | O |
| ATOM | 5191 | C | TYR | 203 | 117.957 | 57.230 | 17.114 | 1.00 | 24.13 | B | C |
| ATOM | 5192 | O | TYR | 203 | 117.268 | 58.211 | 17.387 | 1.00 | 22.30 | B | O |
| ATOM | 5193 | N | SER | 204 | 119.122 | 57.323 | 16.484 | 1.00 | 32.64 | B | N |
| ATOM | 5194 | CA | SER | 204 | 119.693 | 58.608 | 16.089 | 1.00 | 34.49 | B | C |
| ATOM | 5195 | CB | SER | 204 | 121.199 | 58.588 | 16.320 | 1.00 | 50.27 | B | C |
| ATOM | 5196 | OG | SER | 204 | 121.780 | 57.499 | 15.621 | 1.00 | 52.10 | B | O |
| ATOM | 5197 | C | SER | 204 | 119.432 | 58.924 | 14.632 | 1.00 | 37.07 | B | C |
| ATOM | 5198 | O | SER | 204 | 119.922 | 59.919 | 14.118 | 1.00 | 37.58 | B | O |
| ATOM | 5199 | N | SER | 205 | 118.657 | 58.082 | 13.966 | 1.00 | 56.25 | B | N |
| ATOM | 5200 | CA | SER | 205 | 118.379 | 58.289 | 12.558 | 1.00 | 55.91 | B | C |
| ATOM | 5201 | CB | SER | 205 | 119.256 | 57.357 | 11.734 | 1.00 | 30.45 | B | C |
| ATOM | 5202 | OG | SER | 205 | 118.818 | 57.302 | 10.393 | 1.00 | 35.94 | B | O |
| ATOM | 5203 | C | SER | 205 | 116.918 | 58.067 | 12.195 | 1.00 | 54.04 | B | C |
| ATOM | 5204 | O | SER | 205 | 116.208 | 57.320 | 12.866 | 1.00 | 50.30 | B | O |
| ATOM | 5205 | N | THR | 206 | 116.477 | 58.718 | 11.122 | 1.00 | 22.26 | B | N |
| ATOM | 5206 | CA | THR | 206 | 115.105 | 58.589 | 10.661 | 1.00 | 23.61 | B | C |
| ATOM | 5207 | CB | THR | 206 | 114.799 | 59.611 | 9.560 | 1.00 | 36.04 | B | C |
| ATOM | 5208 | OG1 | THR | 206 | 114.968 | 60.935 | 10.086 | 1.00 | 34.85 | B | O |
| ATOM | 5209 | CG2 | THR | 206 | 113.364 | 59.438 | 9.047 | 1.00 | 34.41 | B | C |
| ATOM | 5210 | C | THR | 206 | 114.780 | 57.188 | 10.144 | 1.00 | 24.20 | B | C |
| ATOM | 5211 | O | THR | 206 | 113.676 | 56.683 | 10.363 | 1.00 | 26.99 | B | O |
| ATOM | 5212 | N | GLU | 207 | 115.719 | 56.554 | 9.447 | 1.00 | 31.43 | B | N |
| ATOM | 5213 | CA | GLU | 207 | 115.444 | 55.210 | 8.964 | 1.00 | 30.59 | B | C |
| ATOM | 5214 | CB | GLU | 207 | 116.448 | 54.791 | 7.893 | 1.00 | 74.76 | B | C |
| ATOM | 5215 | CG | GLU | 207 | 117.897 | 54.985 | 8.248 | 1.00 | 75.48 | B | C |
| ATOM | 5216 | CD | GLU | 207 | 118.817 | 54.402 | 7.189 | 1.00 | 76.89 | B | C |
| ATOM | 5217 | OE1 | GLU | 207 | 118.595 | 54.668 | 5.982 | 1.00 | 76.12 | B | O |
| ATOM | 5218 | OE2 | GLU | 207 | 119.765 | 53.679 | 7.565 | 1.00 | 75.79 | B | O |
| ATOM | 5219 | C | GLU | 207 | 115.462 | 54.237 | 10.141 | 1.00 | 31.09 | B | C |
| ATOM | 5220 | O | GLU | 207 | 114.647 | 53.315 | 10.194 | 1.00 | 31.04 | B | O |
| ATOM | 5221 | N | GLU | 208 | 116.373 | 54.449 | 11.093 | 1.00 | 40.73 | B | N |
| ATOM | 5222 | CA | GLU | 208 | 116.441 | 53.584 | 12.267 | 1.00 | 42.46 | B | C |
| ATOM | 5223 | CB | GLU | 208 | 117.542 | 54.038 | 13.230 | 1.00 | 57.02 | B | C |
| ATOM | 5224 | CG | GLU | 208 | 118.951 | 53.899 | 12.682 | 1.00 | 54.49 | B | C |
| ATOM | 5225 | CD | GLU | 208 | 120.022 | 54.254 | 13.703 | 1.00 | 54.01 | B | C |
| ATOM | 5226 | OE1 | GLU | 208 | 121.217 | 54.253 | 13.333 | 1.00 | 59.78 | B | O |
| ATOM | 5227 | OE2 | GLU | 208 | 119.669 | 54.533 | 14.873 | 1.00 | 52.73 | B | O |
| ATOM | 5228 | C | GLU | 208 | 115.100 | 53.611 | 12.991 | 1.00 | 43.16 | B | C |
| ATOM | 5229 | O | GLU | 208 | 114.637 | 52.584 | 13.489 | 1.00 | 44.16 | B | O |
| ATOM | 5230 | N | VAL | 209 | 114.478 | 54.787 | 13.046 | 1.00 | 30.06 | B | N |
| ATOM | 5231 | CA | VAL | 209 | 113.190 | 54.922 | 13.709 | 1.00 | 28.98 | B | C |
| ATOM | 5232 | CB | VAL | 209 | 112.879 | 56.399 | 14.058 | 1.00 | 17.77 | B | C |
| ATOM | 5233 | CG1 | VAL | 209 | 111.379 | 56.612 | 14.232 | 1.00 | 18.10 | B | C |
| ATOM | 5234 | CG2 | VAL | 209 | 113.575 | 56.762 | 15.349 | 1.00 | 18.79 | B | C |
| ATOM | 5235 | C | VAL | 209 | 112.098 | 54.359 | 12.820 | 1.00 | 27.00 | B | C |
| ATOM | 5236 | O | VAL | 209 | 111.198 | 53.660 | 13.296 | 1.00 | 25.96 | B | O |
| ATOM | 5237 | N | LEU | 210 | 112.187 | 54.655 | 11.529 | 1.00 | 33.19 | B | N |
| ATOM | 5238 | CA | LEU | 210 | 111.207 | 54.164 | 10.570 | 1.00 | 33.52 | B | C |
| ATOM | 5239 | CB | LEU | 210 | 111.557 | 54.643 | 9.168 | 1.00 | 15.67 | B | C |
| ATOM | 5240 | CG | LEU | 210 | 110.629 | 55.672 | 8.535 | 1.00 | 15.91 | B | C |
| ATOM | 5241 | CD1 | LEU | 210 | 111.182 | 55.981 | 7.171 | 1.00 | 12.46 | B | C |
| ATOM | 5242 | CD2 | LEU | 210 | 109.191 | 55.157 | 8.437 | 1.00 | 9.36 | B | C |
| ATOM | 5243 | C | LEU | 210 | 111.152 | 52.639 | 10.571 | 1.00 | 31.78 | B | C |
| ATOM | 5244 | O | LEU | 210 | 110.090 | 52.042 | 10.382 | 1.00 | 32.55 | B | O |
| ATOM | 5245 | N | VAL | 211 | 112.307 | 52.017 | 10.779 | 1.00 | 24.37 | B | N |
| ATOM | 5246 | CA | VAL | 211 | 112.404 | 50.569 | 10.809 | 1.00 | 24.13 | B | C |
| ATOM | 5247 | CB | VAL | 211 | 113.852 | 50.123 | 10.575 | 1.00 | 20.01 | B | C |
| ATOM | 5248 | CG1 | VAL | 211 | 114.002 | 48.647 | 10.897 | 1.00 | 22.19 | B | C |
| ATOM | 5249 | CG2 | VAL | 211 | 114.239 | 50.405 | 9.118 | 1.00 | 20.62 | B | C |
| ATOM | 5250 | C | VAL | 211 | 111.913 | 49.997 | 12.129 | 1.00 | 23.38 | B | C |
| ATOM | 5251 | O | VAL | 211 | 111.260 | 48.958 | 12.164 | 1.00 | 24.06 | B | O |
| ATOM | 5252 | N | ALA | 212 | 112.230 | 50.674 | 13.221 | 1.00 | 40.83 | B | N |
| ATOM | 5253 | CA | ALA | 212 | 111.803 | 50.203 | 14.526 | 1.00 | 39.81 | B | C |
| ATOM | 5254 | CB | ALA | 212 | 112.489 | 51.000 | 15.612 | 1.00 | 28.52 | B | C |
| ATOM | 5255 | C | ALA | 212 | 110.295 | 50.339 | 14.650 | 1.00 | 37.62 | B | C |
| ATOM | 5256 | O | ALA | 212 | 109.626 | 49.493 | 15.256 | 1.00 | 37.56 | B | O |

Fig. 19: A-73

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 5257 | N | ALA | 213 | 109.759 | 51.408 | 14.069 | 1.00 | 31.97 | B | N |
| ATOM | 5258 | CA | ALA | 213 | 108.324 | 51.658 | 14.122 | 1.00 | 33.14 | B | C |
| ATOM | 5259 | CB | ALA | 213 | 107.999 | 52.998 | 13.459 | 1.00 | 19.99 | B | C |
| ATOM | 5260 | C | ALA | 213 | 107.530 | 50.535 | 13.458 | 1.00 | 31.94 | B | C |
| ATOM | 5261 | O | ALA | 213 | 106.556 | 50.029 | 14.025 | 1.00 | 29.57 | B | O |
| ATOM | 5262 | N | ASN | 214 | 107.954 | 50.142 | 12.258 | 1.00 | 35.89 | B | N |
| ATOM | 5263 | CA | ASN | 214 | 107.264 | 49.091 | 11.524 | 1.00 | 39.76 | B | C |
| ATOM | 5264 | CB | ASN | 214 | 107.804 | 48.970 | 10.100 | 1.00 | 79.46 | B | C |
| ATOM | 5265 | CG | ASN | 214 | 107.278 | 50.049 | 9.190 | 1.00 | 81.19 | B | C |
| ATOM | 5266 | OD1 | ASN | 214 | 107.668 | 51.210 | 9.296 | 1.00 | 83.12 | B | O |
| ATOM | 5267 | ND2 | ASN | 214 | 106.379 | 49.676 | 8.289 | 1.00 | 81.61 | B | N |
| ATOM | 5268 | C | ASN | 214 | 107.348 | 47.738 | 12.207 | 1.00 | 42.15 | B | C |
| ATOM | 5269 | O | ASN | 214 | 106.583 | 46.829 | 11.891 | 1.00 | 42.87 | B | O |
| ATOM | 5270 | N | LYS | 215 | 108.271 | 47.596 | 13.148 | 1.00 | 30.37 | B | N |
| ATOM | 5271 | CA | LYS | 215 | 108.418 | 46.326 | 13.856 | 1.00 | 30.81 | B | C |
| ATOM | 5272 | CB | LYS | 215 | 109.892 | 46.059 | 14.209 | 1.00 | 46.54 | B | C |
| ATOM | 5273 | CG | LYS | 215 | 110.791 | 45.922 | 12.978 | 1.00 | 54.12 | B | C |
| ATOM | 5274 | CD | LYS | 215 | 112.062 | 45.124 | 13.256 | 1.00 | 57.66 | B | C |
| ATOM | 5275 | CE | LYS | 215 | 112.950 | 45.778 | 14.311 | 1.00 | 61.12 | B | C |
| ATOM | 5276 | NZ | LYS | 215 | 114.249 | 45.057 | 14.488 | 1.00 | 62.11 | B | N |
| ATOM | 5277 | C | LYS | 215 | 107.560 | 46.274 | 15.113 | 1.00 | 28.94 | B | C |
| ATOM | 5278 | O | LYS | 215 | 107.568 | 45.277 | 15.832 | 1.00 | 30.16 | B | O |
| ATOM | 5279 | N | ILE | 216 | 106.809 | 47.341 | 15.377 | 1.00 | 44.32 | B | N |
| ATOM | 5280 | CA | ILE | 216 | 105.945 | 47.362 | 16.553 | 1.00 | 41.14 | B | C |
| ATOM | 5281 | CB | ILE | 216 | 105.443 | 48.776 | 16.874 | 1.00 | 15.33 | B | C |
| ATOM | 5282 | CG2 | ILE | 216 | 104.492 | 48.730 | 18.038 | 1.00 | 12.11 | B | C |
| ATOM | 5283 | CG1 | ILE | 216 | 106.616 | 49.674 | 17.243 | 1.00 | 12.01 | B | C |
| ATOM | 5284 | CD1 | ILE | 216 | 106.191 | 51.073 | 17.602 | 1.00 | 10.70 | B | C |
| ATOM | 5285 | C | ILE | 216 | 104.740 | 46.447 | 16.369 | 1.00 | 39.58 | B | C |
| ATOM | 5286 | O | ILE | 216 | 104.035 | 46.498 | 15.361 | 1.00 | 40.28 | B | O |
| ATOM | 5287 | N | VAL | 217 | 104.524 | 45.611 | 17.372 | 1.00 | 36.13 | B | N |
| ATOM | 5288 | CA | VAL | 217 | 103.436 | 44.647 | 17.392 | 1.00 | 37.90 | B | C |
| ATOM | 5289 | CB | VAL | 217 | 103.949 | 43.284 | 17.887 | 1.00 | 59.95 | B | C |
| ATOM | 5290 | CG1 | VAL | 217 | 102.793 | 42.367 | 18.217 | 1.00 | 59.95 | B | C |
| ATOM | 5291 | CG2 | VAL | 217 | 104.837 | 42.666 | 16.829 | 1.00 | 59.95 | B | C |
| ATOM | 5292 | C | VAL | 217 | 102.316 | 45.111 | 18.311 | 1.00 | 39.06 | B | C |
| ATOM | 5293 | O | VAL | 217 | 102.565 | 45.725 | 19.352 | 1.00 | 38.52 | B | O |
| ATOM | 5294 | N | GLN | 218 | 101.084 | 44.809 | 17.914 | 1.00 | 32.14 | B | N |
| ATOM | 5295 | CA | GLN | 218 | 99.907 | 45.181 | 18.687 | 1.00 | 32.80 | B | C |
| ATOM | 5296 | CB | GLN | 218 | 98.646 | 44.976 | 17.850 | 1.00 | 28.44 | B | C |
| ATOM | 5297 | CG | GLN | 218 | 97.378 | 45.433 | 18.528 | 1.00 | 28.44 | B | C |
| ATOM | 5298 | CD | GLN | 218 | 96.153 | 45.273 | 17.644 | 1.00 | 28.44 | B | C |
| ATOM | 5299 | OE1 | GLN | 218 | 95.096 | 45.843 | 17.928 | 1.00 | 28.44 | B | O |
| ATOM | 5300 | NE2 | GLN | 218 | 96.283 | 44.490 | 16.571 | 1.00 | 28.44 | B | N |
| ATOM | 5301 | C | GLN | 218 | 99.856 | 44.288 | 19.913 | 1.00 | 32.25 | B | C |
| ATOM | 5302 | O | GLN | 218 | 99.948 | 43.079 | 19.792 | 1.00 | 36.00 | B | O |
| ATOM | 5303 | N | ARG | 219 | 99.709 | 44.883 | 21.091 | 1.00 | 14.17 | B | N |
| ATOM | 5304 | CA | ARG | 219 | 99.664 | 44.114 | 22.330 | 1.00 | 13.82 | B | C |
| ATOM | 5305 | CB | ARG | 219 | 100.490 | 44.828 | 23.394 | 1.00 | 43.11 | B | C |
| ATOM | 5306 | CG | ARG | 219 | 101.627 | 45.640 | 22.823 | 1.00 | 43.11 | B | C |
| ATOM | 5307 | CD | ARG | 219 | 102.594 | 46.039 | 23.901 | 1.00 | 43.11 | B | C |
| ATOM | 5308 | NE | ARG | 219 | 103.597 | 45.007 | 24.124 | 1.00 | 43.11 | B | N |
| ATOM | 5309 | CZ | ARG | 219 | 104.694 | 44.867 | 23.384 | 1.00 | 43.11 | B | C |
| ATOM | 5310 | NH1 | ARG | 219 | 104.921 | 45.705 | 22.369 | 1.00 | 43.11 | B | N |
| ATOM | 5311 | NH2 | ARG | 219 | 105.566 | 43.900 | 23.661 | 1.00 | 43.11 | B | N |
| ATOM | 5312 | C | ARG | 219 | 98.221 | 43.910 | 22.821 | 1.00 | 15.03 | B | C |
| ATOM | 5313 | O | ARG | 219 | 97.976 | 43.309 | 23.871 | 1.00 | 15.04 | B | O |
| ATOM | 5314 | N | GLY | 220 | 97.269 | 44.423 | 22.048 | 1.00 | 30.91 | B | N |
| ATOM | 5315 | CA | GLY | 220 | 95.868 | 44.283 | 22.402 | 1.00 | 30.52 | B | C |
| ATOM | 5316 | C | GLY | 220 | 95.495 | 44.884 | 23.742 | 1.00 | 30.19 | B | C |
| ATOM | 5317 | O | GLY | 220 | 96.246 | 45.674 | 24.327 | 1.00 | 28.53 | B | O |
| ATOM | 5318 | N | GLY | 221 | 94.316 | 44.511 | 24.222 | 1.00 | 22.15 | B | N |
| ATOM | 5319 | CA | GLY | 221 | 93.852 | 45.009 | 25.500 | 1.00 | 20.72 | B | C |
| ATOM | 5320 | C | GLY | 221 | 92.348 | 44.902 | 25.652 | 1.00 | 21.14 | B | C |
| ATOM | 5321 | O | GLY | 221 | 91.598 | 45.328 | 24.776 | 1.00 | 17.94 | B | O |
| ATOM | 5322 | N | ARG | 222 | 91.897 | 44.327 | 26.760 | 1.00 | 28.36 | B | N |
| ATOM | 5323 | CA | ARG | 222 | 90.467 | 44.199 | 27.011 | 1.00 | 29.07 | B | C |
| ATOM | 5324 | CB | ARG | 222 | 90.204 | 43.114 | 28.053 | 1.00 | 26.86 | B | C |
| ATOM | 5325 | CG | ARG | 222 | 90.365 | 41.713 | 27.491 | 1.00 | 26.86 | B | C |
| ATOM | 5326 | CD | ARG | 222 | 90.427 | 40.663 | 28.578 | 1.00 | 26.86 | B | C |
| ATOM | 5327 | NE | ARG | 222 | 91.679 | 40.734 | 29.316 | 1.00 | 26.86 | B | N |
| ATOM | 5328 | CZ | ARG | 222 | 92.021 | 39.885 | 30.274 | 1.00 | 26.86 | B | C |
| ATOM | 5329 | NH1 | ARG | 222 | 91.201 | 38.895 | 30.612 | 1.00 | 26.86 | B | N |

# Fig. 19: A-74

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 5330 | NH2 | ARG | 222 | 93.184 | 40.027 | 30.893 | 1.00 | 26.86 | B | N |
| ATOM | 5331 | C | ARG | 222 | 89.899 | 45.529 | 27.482 | 1.00 | 29.12 | B | C |
| ATOM | 5332 | O | ARG | 222 | 88.686 | 45.686 | 27.599 | 1.00 | 29.89 | B | O |
| ATOM | 5333 | N | GLN | 223 | 90.792 | 46.477 | 27.756 | 1.00 | 34.74 | B | N |
| ATOM | 5334 | CA | GLN | 223 | 90.423 | 47.826 | 28.182 | 1.00 | 33.03 | B | C |
| ATOM | 5335 | CB | GLN | 223 | 90.700 | 48.050 | 29.677 | 1.00 | 36.16 | B | C |
| ATOM | 5336 | CG | GLN | 223 | 89.723 | 47.394 | 30.641 | 1.00 | 37.60 | B | C |
| ATOM | 5337 | CD | GLN | 223 | 90.065 | 45.957 | 30.915 | 1.00 | 38.01 | B | C |
| ATOM | 5338 | OE1 | GLN | 223 | 91.209 | 45.635 | 31.230 | 1.00 | 38.41 | B | O |
| ATOM | 5339 | NE2 | GLN | 223 | 89.075 | 45.080 | 30.811 | 1.00 | 38.45 | B | N |
| ATOM | 5340 | C | GLN | 223 | 91.221 | 48.849 | 27.372 | 1.00 | 33.77 | B | C |
| ATOM | 5341 | O | GLN | 223 | 92.122 | 48.487 | 26.619 | 1.00 | 33.25 | B | O |
| ATOM | 5342 | N | THR | 224 | 90.893 | 50.126 | 27.535 | 1.00 | 56.95 | B | N |
| ATOM | 5343 | CA | THR | 224 | 91.572 | 51.197 | 26.820 | 1.00 | 54.83 | B | C |
| ATOM | 5344 | CB | THR | 224 | 90.628 | 51.834 | 25.793 | 1.00 | 7.14 | B | C |
| ATOM | 5345 | OG1 | THR | 224 | 90.118 | 50.811 | 24.930 | 1.00 | 7.13 | B | O |
| ATOM | 5346 | CG2 | THR | 224 | 91.357 | 52.895 | 24.965 | 1.00 | 4.73 | B | C |
| ATOM | 5347 | C | THR | 224 | 92.002 | 52.252 | 27.829 | 1.00 | 51.84 | B | C |
| ATOM | 5348 | O | THR | 224 | 91.290 | 53.221 | 28.067 | 1.00 | 48.33 | B | O |
| ATOM | 5349 | N | MET | 225 | 93.175 | 52.061 | 28.419 | 1.00 | 27.08 | B | N |
| ATOM | 5350 | CA | MET | 225 | 93.679 | 52.980 | 29.426 | 1.00 | 27.97 | B | C |
| ATOM | 5351 | CB | MET | 225 | 94.712 | 52.269 | 30.301 | 1.00 | 32.79 | B | C |
| ATOM | 5352 | CG | MET | 225 | 94.280 | 50.904 | 30.804 | 1.00 | 30.22 | B | C |
| ATOM | 5353 | SD | MET | 225 | 92.971 | 50.963 | 31.995 | 1.00 | 37.96 | B | S |
| ATOM | 5354 | CE | MET | 225 | 93.153 | 49.343 | 32.760 | 1.00 | 34.54 | B | C |
| ATOM | 5355 | C | MET | 225 | 94.304 | 54.237 | 28.846 | 1.00 | 29.00 | B | C |
| ATOM | 5356 | O | MET | 225 | 95.442 | 54.561 | 29.180 | 1.00 | 30.46 | B | O |
| ATOM | 5357 | N | THR | 226 | 93.571 | 54.953 | 27.997 | 1.00 | 32.08 | B | N |
| ATOM | 5358 | CA | THR | 226 | 94.102 | 56.178 | 27.393 | 1.00 | 31.55 | B | C |
| ATOM | 5359 | CB | THR | 226 | 93.013 | 56.963 | 26.655 | 1.00 | 28.80 | B | C |
| ATOM | 5360 | OG1 | THR | 226 | 92.395 | 56.132 | 25.665 | 1.00 | 30.82 | B | O |
| ATOM | 5361 | CG2 | THR | 226 | 93.620 | 58.170 | 25.976 | 1.00 | 26.52 | B | C |
| ATOM | 5362 | C | THR | 226 | 94.735 | 57.104 | 28.438 | 1.00 | 30.15 | B | C |
| ATOM | 5363 | O | THR | 226 | 95.804 | 57.672 | 28.216 | 1.00 | 24.84 | B | O |
| ATOM | 5364 | N | ALA | 227 | 94.075 | 57.249 | 29.581 | 1.00 | 17.95 | B | N |
| ATOM | 5365 | CA | ALA | 227 | 94.594 | 58.094 | 30.645 | 1.00 | 16.89 | B | C |
| ATOM | 5366 | CB | ALA | 227 | 93.655 | 58.069 | 31.829 | 1.00 | 18.36 | B | C |
| ATOM | 5367 | C | ALA | 227 | 95.975 | 57.633 | 31.076 | 1.00 | 17.55 | B | C |
| ATOM | 5368 | O | ALA | 227 | 96.898 | 58.439 | 31.199 | 1.00 | 18.35 | B | O |
| ATOM | 5369 | N | LEU | 228 | 96.111 | 56.331 | 31.307 | 1.00 | 19.16 | B | N |
| ATOM | 5370 | CA | LEU | 228 | 97.384 | 55.752 | 31.728 | 1.00 | 17.60 | B | C |
| ATOM | 5371 | CB | LEU | 228 | 97.206 | 54.252 | 32.017 | 1.00 | 6.84 | B | C |
| ATOM | 5372 | CG | LEU | 228 | 98.453 | 53.498 | 32.483 | 1.00 | 14.73 | B | C |
| ATOM | 5373 | CD1 | LEU | 228 | 99.020 | 54.157 | 33.734 | 1.00 | 12.32 | B | C |
| ATOM | 5374 | CD2 | LEU | 228 | 98.097 | 52.064 | 32.732 | 1.00 | 11.78 | B | C |
| ATOM | 5375 | C | LEU | 228 | 98.463 | 55.955 | 30.662 | 1.00 | 16.78 | B | C |
| ATOM | 5376 | O | LEU | 228 | 99.605 | 56.321 | 30.971 | 1.00 | 19.76 | B | O |
| ATOM | 5377 | N | GLY | 229 | 98.094 | 55.713 | 29.408 | 1.00 | 21.79 | B | N |
| ATOM | 5378 | CA | GLY | 229 | 99.033 | 55.877 | 28.318 | 1.00 | 24.15 | B | C |
| ATOM | 5379 | C | GLY | 229 | 99.620 | 57.267 | 28.293 | 1.00 | 26.71 | B | C |
| ATOM | 5380 | O | GLY | 229 | 100.843 | 57.422 | 28.296 | 1.00 | 27.30 | B | O |
| ATOM | 5381 | N | ILE | 230 | 98.756 | 58.281 | 28.280 | 1.00 | 20.54 | B | N |
| ATOM | 5382 | CA | ILE | 230 | 99.216 | 59.666 | 28.259 | 1.00 | 21.87 | B | C |
| ATOM | 5383 | CB | ILE | 230 | 98.039 | 60.677 | 28.160 | 1.00 | 18.79 | B | C |
| ATOM | 5384 | CG2 | ILE | 230 | 98.595 | 62.090 | 28.034 | 1.00 | 18.79 | B | C |
| ATOM | 5385 | CG1 | ILE | 230 | 97.174 | 60.370 | 26.933 | 1.00 | 18.79 | B | C |
| ATOM | 5386 | CD1 | ILE | 230 | 95.945 | 61.225 | 26.807 | 1.00 | 18.79 | B | C |
| ATOM | 5387 | C | ILE | 230 | 100.042 | 60.007 | 29.505 | 1.00 | 22.13 | B | C |
| ATOM | 5388 | O | ILE | 230 | 101.101 | 60.634 | 29.402 | 1.00 | 20.06 | B | O |
| ATOM | 5389 | N | ASP | 231 | 99.566 | 59.595 | 30.677 | 1.00 | 30.92 | B | N |
| ATOM | 5390 | CA | ASP | 231 | 100.286 | 59.876 | 31.916 | 1.00 | 29.32 | B | C |
| ATOM | 5391 | CB | ASP | 231 | 99.494 | 59.354 | 33.116 | 1.00 | 27.91 | B | C |
| ATOM | 5392 | CG | ASP | 231 | 99.993 | 59.917 | 34.442 | 1.00 | 34.91 | B | C |
| ATOM | 5393 | OD1 | ASP | 231 | 99.939 | 61.155 | 34.644 | 1.00 | 33.67 | B | O |
| ATOM | 5394 | OD2 | ASP | 231 | 100.432 | 59.112 | 35.288 | 1.00 | 38.45 | B | O |
| ATOM | 5395 | C | ASP | 231 | 101.676 | 59.231 | 31.884 | 1.00 | 30.30 | B | C |
| ATOM | 5396 | O | ASP | 231 | 102.669 | 59.838 | 32.318 | 1.00 | 27.52 | B | O |
| ATOM | 5397 | N | THR | 232 | 101.741 | 58.007 | 31.361 | 1.00 | 43.37 | B | N |
| ATOM | 5398 | CA | THR | 232 | 102.998 | 57.276 | 31.260 | 1.00 | 42.16 | B | C |
| ATOM | 5399 | CB | THR | 232 | 102.768 | 55.830 | 30.801 | 1.00 | 59.43 | B | C |
| ATOM | 5400 | OG1 | THR | 232 | 101.963 | 55.148 | 31.771 | 1.00 | 57.94 | B | O |
| ATOM | 5401 | CG2 | THR | 232 | 104.097 | 55.098 | 30.645 | 1.00 | 52.97 | B | C |
| ATOM | 5402 | C | THR | 232 | 103.939 | 57.959 | 30.274 | 1.00 | 42.79 | B | C |

Fig. 19: A-75

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 5403 | O | THR | 232 | 105.153 | 58.050 | 30.509 | 1.00 | 42.96 | B | O |
| ATOM | 5404 | N | ALA | 233 | 103.383 | 58.427 | 29.161 | 1.00 | 22.02 | B | N |
| ATOM | 5405 | CA | ALA | 233 | 104.202 | 59.116 | 28.179 | 1.00 | 24.67 | B | C |
| ATOM | 5406 | CB | ALA | 233 | 103.373 | 59.472 | 26.961 | 1.00 | 49.88 | B | C |
| ATOM | 5407 | C | ALA | 233 | 104.752 | 60.385 | 28.836 | 1.00 | 26.98 | B | C |
| ATOM | 5408 | O | ALA | 233 | 105.862 | 60.834 | 28.532 | 1.00 | 28.89 | B | O |
| ATOM | 5409 | N | ARG | 234 | 103.967 | 60.947 | 29.751 | 1.00 | 50.27 | B | N |
| ATOM | 5410 | CA | ARG | 234 | 104.361 | 62.165 | 30.431 | 1.00 | 53.37 | B | C |
| ATOM | 5411 | CB | ARG | 234 | 103.146 | 62.842 | 31.077 | 1.00 | 50.29 | B | C |
| ATOM | 5412 | CG | ARG | 234 | 103.377 | 64.312 | 31.390 | 1.00 | 50.29 | B | C |
| ATOM | 5413 | CD | ARG | 234 | 102.536 | 64.816 | 32.561 | 1.00 | 50.29 | B | C |
| ATOM | 5414 | NE | ARG | 234 | 103.103 | 64.432 | 33.852 | 1.00 | 50.29 | B | N |
| ATOM | 5415 | CZ | ARG | 234 | 102.668 | 63.418 | 34.592 | 1.00 | 50.29 | B | C |
| ATOM | 5416 | NH1 | ARG | 234 | 101.650 | 62.682 | 34.172 | 1.00 | 50.29 | B | N |
| ATOM | 5417 | NH2 | ARG | 234 | 103.258 | 63.135 | 35.744 | 1.00 | 50.29 | B | N |
| ATOM | 5418 | C | ARG | 234 | 105.406 | 61.904 | 31.498 | 1.00 | 55.50 | B | C |
| ATOM | 5419 | O | ARG | 234 | 106.556 | 62.316 | 31.368 | 1.00 | 55.55 | B | O |
| ATOM | 5420 | N | LYS | 235 | 105.009 | 61.196 | 32.547 | 1.00 | 27.28 | B | N |
| ATOM | 5421 | CA | LYS | 235 | 105.914 | 60.939 | 33.660 | 1.00 | 27.23 | B | C |
| ATOM | 5422 | CB | LYS | 235 | 105.129 | 60.356 | 34.848 | 1.00 | 39.45 | B | C |
| ATOM | 5423 | CG | LYS | 235 | 104.888 | 58.857 | 34.831 | 1.00 | 40.60 | B | C |
| ATOM | 5424 | CD | LYS | 235 | 104.027 | 58.450 | 36.030 | 1.00 | 40.42 | B | C |
| ATOM | 5425 | CE | LYS | 235 | 104.119 | 56.955 | 36.346 | 1.00 | 41.22 | B | C |
| ATOM | 5426 | NZ | LYS | 235 | 103.715 | 56.073 | 35.205 | 1.00 | 41.98 | B | N |
| ATOM | 5427 | C | LYS | 235 | 107.149 | 60.078 | 33.375 | 1.00 | 27.37 | B | C |
| ATOM | 5428 | O | LYS | 235 | 108.112 | 60.118 | 34.130 | 1.00 | 27.71 | B | O |
| ATOM | 5429 | N | GLU | 236 | 107.133 | 59.313 | 32.290 | 1.00 | 28.33 | B | N |
| ATOM | 5430 | CA | GLU | 236 | 108.264 | 58.454 | 31.964 | 1.00 | 29.95 | B | C |
| ATOM | 5431 | CB | GLU | 236 | 107.803 | 56.992 | 31.884 | 1.00 | 47.54 | B | C |
| ATOM | 5432 | CG | GLU | 236 | 107.861 | 56.249 | 33.216 | 1.00 | 50.31 | B | C |
| ATOM | 5433 | CD | GLU | 236 | 107.031 | 54.965 | 33.245 | 1.00 | 52.79 | B | C |
| ATOM | 5434 | OE1 | GLU | 236 | 107.194 | 54.118 | 32.342 | 1.00 | 52.88 | B | O |
| ATOM | 5435 | OE2 | GLU | 236 | 106.219 | 54.797 | 34.184 | 1.00 | 52.63 | B | O |
| ATOM | 5436 | C | GLU | 236 | 108.966 | 58.840 | 30.670 | 1.00 | 28.50 | B | C |
| ATOM | 5437 | O | GLU | 236 | 110.092 | 59.336 | 30.684 | 1.00 | 29.93 | B | O |
| ATOM | 5438 | N | ALA | 237 | 108.287 | 58.617 | 29.552 | 1.00 | 22.73 | B | N |
| ATOM | 5439 | CA | ALA | 237 | 108.860 | 58.901 | 28.248 | 1.00 | 20.20 | B | C |
| ATOM | 5440 | CB | ALA | 237 | 107.783 | 58.831 | 27.180 | 1.00 | 41.37 | B | C |
| ATOM | 5441 | C | ALA | 237 | 109.562 | 60.233 | 28.187 | 1.00 | 19.04 | B | C |
| ATOM | 5442 | O | ALA | 237 | 110.636 | 60.344 | 27.589 | 1.00 | 17.46 | B | O |
| ATOM | 5443 | N | PHE | 238 | 108.962 | 61.242 | 28.810 | 1.00 | 29.57 | B | N |
| ATOM | 5444 | CA | PHE | 238 | 109.530 | 62.580 | 28.795 | 1.00 | 29.00 | B | C |
| ATOM | 5445 | CB | PHE | 238 | 108.419 | 63.620 | 28.752 | 1.00 | 35.30 | B | C |
| ATOM | 5446 | CG | PHE | 238 | 107.856 | 63.854 | 27.381 | 1.00 | 34.33 | B | C |
| ATOM | 5447 | CD1 | PHE | 238 | 106.531 | 63.532 | 27.101 | 1.00 | 35.56 | B | C |
| ATOM | 5448 | CD2 | PHE | 238 | 108.635 | 64.429 | 26.380 | 1.00 | 31.93 | B | C |
| ATOM | 5449 | CE1 | PHE | 238 | 105.985 | 63.780 | 25.841 | 1.00 | 33.36 | B | C |
| ATOM | 5450 | CE2 | PHE | 238 | 108.106 | 64.682 | 25.124 | 1.00 | 38.24 | B | C |
| ATOM | 5451 | CZ | PHE | 238 | 106.778 | 64.359 | 24.850 | 1.00 | 39.66 | B | C |
| ATOM | 5452 | C | PHE | 238 | 110.468 | 62.908 | 29.943 | 1.00 | 30.85 | B | C |
| ATOM | 5453 | O | PHE | 238 | 110.433 | 64.012 | 30.479 | 1.00 | 30.95 | B | O |
| ATOM | 5454 | N | THR | 239 | 111.303 | 61.951 | 30.325 | 1.00 | 29.27 | B | N |
| ATOM | 5455 | CA | THR | 239 | 112.266 | 62.182 | 31.391 | 1.00 | 33.21 | B | C |
| ATOM | 5456 | CB | THR | 239 | 112.113 | 61.150 | 32.520 | 1.00 | 23.55 | B | C |
| ATOM | 5457 | OG1 | THR | 239 | 112.276 | 59.840 | 31.989 | 1.00 | 21.51 | B | O |
| ATOM | 5458 | CG2 | THR | 239 | 110.745 | 61.242 | 33.153 | 1.00 | 26.46 | B | C |
| ATOM | 5459 | C | THR | 239 | 113.660 | 62.084 | 30.770 | 1.00 | 33.47 | B | C |
| ATOM | 5460 | O | THR | 239 | 113.930 | 61.177 | 29.980 | 1.00 | 33.97 | B | O |
| ATOM | 5461 | N | GLU | 240 | 114.531 | 63.030 | 31.117 | 1.00 | 17.24 | B | N |
| ATOM | 5462 | CA | GLU | 240 | 115.890 | 63.085 | 30.580 | 1.00 | 17.49 | B | C |
| ATOM | 5463 | CB | GLU | 240 | 116.748 | 64.003 | 31.444 | 1.00 | 74.12 | B | C |
| ATOM | 5464 | CG | GLU | 240 | 118.007 | 64.483 | 30.758 | 1.00 | 78.76 | B | C |
| ATOM | 5465 | CD | GLU | 240 | 118.634 | 65.654 | 31.479 | 1.00 | 81.67 | B | C |
| ATOM | 5466 | OE1 | GLU | 240 | 117.904 | 66.627 | 31.774 | 1.00 | 81.77 | B | O |
| ATOM | 5467 | OE2 | GLU | 240 | 119.853 | 65.605 | 31.746 | 1.00 | 81.74 | B | O |
| ATOM | 5468 | C | GLU | 240 | 116.555 | 61.712 | 30.465 | 1.00 | 18.84 | B | C |
| ATOM | 5469 | O | GLU | 240 | 117.323 | 61.444 | 29.530 | 1.00 | 20.05 | B | O |
| ATOM | 5470 | N | ALA | 241 | 116.234 | 60.839 | 31.415 | 1.00 | 54.75 | B | N |
| ATOM | 5471 | CA | ALA | 241 | 116.784 | 59.491 | 31.446 | 1.00 | 55.60 | B | C |
| ATOM | 5472 | CB | ALA | 241 | 116.331 | 58.783 | 32.723 | 1.00 | 26.00 | B | C |
| ATOM | 5473 | C | ALA | 241 | 116.387 | 58.678 | 30.212 | 1.00 | 55.07 | B | C |
| ATOM | 5474 | O | ALA | 241 | 117.093 | 57.751 | 29.823 | 1.00 | 56.53 | B | O |
| ATOM | 5475 | N | ARG | 242 | 115.259 | 59.024 | 29.598 | 1.00 | 25.17 | B | N |

Fig. 19: A-76

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 5476 | CA | ARG | 242 | 114.805 | 58.305 | 28.417 | 1.00 | 24.91 | B | C |
| ATOM | 5477 | CB | ARG | 242 | 113.337 | 57.917 | 28.570 | 1.00 | 45.62 | B | C |
| ATOM | 5478 | CG | ARG | 242 | 113.136 | 56.644 | 29.392 | 1.00 | 45.82 | B | C |
| ATOM | 5479 | CD | ARG | 242 | 111.684 | 56.188 | 29.334 | 1.00 | 46.68 | B | C |
| ATOM | 5480 | NE | ARG | 242 | 111.525 | 54.733 | 29.424 | 1.00 | 47.88 | B | N |
| ATOM | 5481 | CZ | ARG | 242 | 111.348 | 54.055 | 30.557 | 1.00 | 47.08 | B | C |
| ATOM | 5482 | NH1 | ARG | 242 | 111.307 | 54.695 | 31.721 | 1.00 | 46.13 | B | N |
| ATOM | 5483 | NH2 | ARG | 242 | 111.187 | 52.738 | 30.526 | 1.00 | 49.10 | B | N |
| ATOM | 5484 | C | ARG | 242 | 115.039 | 59.088 | 27.120 | 1.00 | 26.11 | B | C |
| ATOM | 5485 | O | ARG | 242 | 114.450 | 58.796 | 26.076 | 1.00 | 29.12 | B | O |
| ATOM | 5486 | N | GLY | 243 | 115.919 | 60.079 | 27.194 | 1.00 | 41.48 | B | N |
| ATOM | 5487 | CA | GLY | 243 | 116.226 | 60.863 | 26.014 | 1.00 | 39.63 | B | C |
| ATOM | 5488 | C | GLY | 243 | 115.497 | 62.187 | 25.893 | 1.00 | 37.91 | B | C |
| ATOM | 5489 | O | GLY | 243 | 115.454 | 62.774 | 24.810 | 1.00 | 37.53 | B | O |
| ATOM | 5490 | N | ALA | 244 | 114.913 | 62.665 | 26.986 | 1.00 | 32.61 | B | N |
| ATOM | 5491 | CA | ALA | 244 | 114.209 | 63.941 | 26.939 | 1.00 | 30.61 | B | C |
| ATOM | 5492 | CB | ALA | 244 | 113.253 | 64.074 | 28.124 | 1.00 | 2.29 | B | C |
| ATOM | 5493 | C | ALA | 244 | 115.262 | 65.033 | 26.984 | 1.00 | 32.49 | B | C |
| ATOM | 5494 | O | ALA | 244 | 115.867 | 65.266 | 28.021 | 1.00 | 31.95 | B | O |
| ATOM | 5495 | N | ARG | 245 | 115.491 | 65.690 | 25.854 | 1.00 | 46.10 | B | N |
| ATOM | 5496 | CA | ARG | 245 | 116.482 | 66.760 | 25.768 | 1.00 | 46.93 | B | C |
| ATOM | 5497 | CB | ARG | 245 | 116.690 | 67.163 | 24.309 | 1.00 | 24.44 | B | C |
| ATOM | 5498 | CG | ARG | 245 | 117.460 | 66.126 | 23.503 | 1.00 | 26.91 | B | C |
| ATOM | 5499 | CD | ARG | 245 | 117.553 | 66.517 | 22.054 | 1.00 | 27.12 | B | C |
| ATOM | 5500 | NE | ARG | 245 | 116.229 | 66.560 | 21.457 | 1.00 | 21.54 | B | N |
| ATOM | 5501 | CZ | ARG | 245 | 115.999 | 66.826 | 20.179 | 1.00 | 21.36 | B | C |
| ATOM | 5502 | NH1 | ARG | 245 | 117.016 | 67.074 | 19.370 | 1.00 | 20.56 | B | N |
| ATOM | 5503 | NH2 | ARG | 245 | 114.756 | 66.834 | 19.708 | 1.00 | 18.65 | B | N |
| ATOM | 5504 | C | ARG | 245 | 116.101 | 67.986 | 26.585 | 1.00 | 45.30 | B | C |
| ATOM | 5505 | O | ARG | 245 | 114.975 | 68.480 | 26.496 | 1.00 | 41.41 | B | O |
| ATOM | 5506 | N | ARG | 246 | 117.051 | 68.476 | 27.376 | 1.00 | 48.54 | B | N |
| ATOM | 5507 | CA | ARG | 246 | 116.830 | 69.640 | 28.229 | 1.00 | 51.33 | B | C |
| ATOM | 5508 | CB | ARG | 246 | 118.096 | 69.982 | 29.012 | 1.00 | 83.48 | B | C |
| ATOM | 5509 | CG | ARG | 246 | 117.975 | 71.269 | 29.811 | 1.00 | 88.84 | B | C |
| ATOM | 5510 | CD | ARG | 246 | 119.295 | 71.647 | 30.449 | 1.00 | 94.76 | B | C |
| ATOM | 5511 | NE | ARG | 246 | 119.896 | 70.525 | 31.165 | 1.00 | 97.67 | B | N |
| ATOM | 5512 | CZ | ARG | 246 | 119.288 | 69.828 | 32.123 | 1.00 | 100.78 | B | C |
| ATOM | 5513 | NH1 | ARG | 246 | 118.047 | 70.132 | 32.491 | 1.00 | 100.47 | B | N |
| ATOM | 5514 | NH2 | ARG | 246 | 119.923 | 68.825 | 32.717 | 1.00 | 101.56 | B | N |
| ATOM | 5515 | C | ARG | 246 | 116.415 | 70.871 | 27.448 | 1.00 | 49.15 | B | C |
| ATOM | 5516 | O | ARG | 246 | 117.082 | 71.246 | 26.489 | 1.00 | 51.78 | B | O |
| ATOM | 5517 | N | GLY | 247 | 115.311 | 71.489 | 27.868 | 1.00 | 46.59 | B | N |
| ATOM | 5518 | CA | GLY | 247 | 114.825 | 72.705 | 27.233 | 1.00 | 49.17 | B | C |
| ATOM | 5519 | C | GLY | 247 | 114.381 | 72.609 | 25.787 | 1.00 | 49.24 | B | C |
| ATOM | 5520 | O | GLY | 247 | 114.531 | 73.560 | 25.019 | 1.00 | 52.20 | B | O |
| ATOM | 5521 | N | VAL | 248 | 113.836 | 71.462 | 25.407 | 1.00 | 57.57 | B | N |
| ATOM | 5522 | CA | VAL | 248 | 113.357 | 71.266 | 24.049 | 1.00 | 55.58 | B | C |
| ATOM | 5523 | CB | VAL | 248 | 114.012 | 70.043 | 23.407 | 1.00 | 22.85 | B | C |
| ATOM | 5524 | CG1 | VAL | 248 | 113.384 | 69.765 | 22.056 | 1.00 | 20.50 | B | C |
| ATOM | 5525 | CG2 | VAL | 248 | 115.499 | 70.287 | 23.266 | 1.00 | 14.62 | B | C |
| ATOM | 5526 | C | VAL | 248 | 111.855 | 71.056 | 24.094 | 1.00 | 58.60 | B | C |
| ATOM | 5527 | O | VAL | 248 | 111.343 | 70.403 | 25.005 | 1.00 | 62.65 | B | O |
| ATOM | 5528 | N | LYS | 249 | 111.147 | 71.607 | 23.115 | 1.00 | 37.34 | B | N |
| ATOM | 5529 | CA | LYS | 249 | 109.698 | 71.464 | 23.086 | 1.00 | 38.25 | B | C |
| ATOM | 5530 | CB | LYS | 249 | 109.115 | 72.122 | 21.832 | 1.00 | 57.29 | B | C |
| ATOM | 5531 | CG | LYS | 249 | 107.594 | 72.204 | 21.869 | 1.00 | 62.81 | B | C |
| ATOM | 5532 | CD | LYS | 249 | 107.103 | 72.892 | 23.155 | 1.00 | 63.88 | B | C |
| ATOM | 5533 | CE | LYS | 249 | 105.634 | 72.579 | 23.450 | 1.00 | 66.24 | B | C |
| ATOM | 5534 | NZ | LYS | 249 | 105.067 | 73.292 | 24.636 | 1.00 | 69.06 | B | N |
| ATOM | 5535 | C | LYS | 249 | 109.244 | 69.998 | 23.173 | 1.00 | 36.91 | B | C |
| ATOM | 5536 | O | LYS | 249 | 109.790 | 69.112 | 22.505 | 1.00 | 36.73 | B | O |
| ATOM | 5537 | N | LYS | 250 | 108.238 | 69.755 | 24.009 | 1.00 | 33.42 | B | N |
| ATOM | 5538 | CA | LYS | 250 | 107.706 | 68.419 | 24.208 | 1.00 | 33.07 | B | C |
| ATOM | 5539 | CB | LYS | 250 | 107.603 | 68.147 | 25.710 | 1.00 | 46.37 | B | C |
| ATOM | 5540 | CG | LYS | 250 | 108.970 | 68.151 | 26.374 | 1.00 | 44.97 | B | C |
| ATOM | 5541 | CD | LYS | 250 | 108.918 | 68.429 | 27.872 | 1.00 | 46.52 | B | C |
| ATOM | 5542 | CE | LYS | 250 | 108.389 | 67.256 | 28.686 | 1.00 | 45.68 | B | C |
| ATOM | 5543 | NZ | LYS | 250 | 108.578 | 67.474 | 30.157 | 1.00 | 47.50 | B | N |
| ATOM | 5544 | C | LYS | 250 | 106.355 | 68.263 | 23.506 | 1.00 | 32.42 | B | C |
| ATOM | 5545 | O | LYS | 250 | 105.380 | 68.931 | 23.842 | 1.00 | 32.10 | B | O |
| ATOM | 5546 | N | VAL | 251 | 106.320 | 67.372 | 22.519 | 1.00 | 37.83 | B | N |
| ATOM | 5547 | CA | VAL | 251 | 105.121 | 67.115 | 21.730 | 1.00 | 37.74 | B | C |
| ATOM | 5548 | CB | VAL | 251 | 105.403 | 67.373 | 20.248 | 1.00 | 28.71 | B | C |

Fig. 19: A-77

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 5549 | CG1 | VAL | 251 | 104.180 | 67.017 | 19.410 | 1.00 | 26.86 | B | C |
| ATOM | 5550 | CG2 | VAL | 251 | 105.819 | 68.822 | 20.057 | 1.00 | 29.92 | B | C |
| ATOM | 5551 | C | VAL | 251 | 104.591 | 65.689 | 21.866 | 1.00 | 36.22 | B | C |
| ATOM | 5552 | O | VAL | 251 | 105.339 | 64.715 | 21.714 | 1.00 | 32.22 | B | O |
| ATOM | 5553 | N | MET | 252 | 103.289 | 65.572 | 22.122 | 1.00 | 42.57 | B | N |
| ATOM | 5554 | CA | MET | 252 | 102.651 | 64.269 | 22.275 | 1.00 | 43.55 | B | C |
| ATOM | 5555 | CB | MET | 252 | 102.013 | 64.160 | 23.660 | 1.00 | 27.32 | B | C |
| ATOM | 5556 | CG | MET | 252 | 101.440 | 62.787 | 23.998 | 1.00 | 26.01 | B | C |
| ATOM | 5557 | SD | MET | 252 | 100.740 | 62.725 | 25.675 | 1.00 | 30.06 | B | S |
| ATOM | 5558 | CE | MET | 252 | 102.222 | 63.011 | 26.691 | 1.00 | 21.37 | B | C |
| ATOM | 5559 | C | MET | 252 | 101.583 | 64.060 | 21.217 | 1.00 | 42.57 | B | C |
| ATOM | 5560 | O | MET | 252 | 100.761 | 64.937 | 20.982 | 1.00 | 44.94 | B | O |
| ATOM | 5561 | N | VAL | 253 | 101.604 | 62.900 | 20.573 | 1.00 | 21.89 | B | N |
| ATOM | 5562 | CA | VAL | 253 | 100.607 | 62.580 | 19.558 | 1.00 | 23.04 | B | C |
| ATOM | 5563 | CB | VAL | 253 | 101.267 | 62.281 | 18.187 | 1.00 | 9.79 | B | C |
| ATOM | 5564 | CG1 | VAL | 253 | 100.191 | 61.900 | 17.168 | 1.00 | 11.21 | B | C |
| ATOM | 5565 | CG2 | VAL | 253 | 102.044 | 63.490 | 17.701 | 1.00 | 9.43 | B | C |
| ATOM | 5566 | C | VAL | 253 | 99.819 | 61.353 | 20.015 | 1.00 | 22.61 | B | C |
| ATOM | 5567 | O | VAL | 253 | 100.383 | 60.276 | 20.161 | 1.00 | 21.05 | B | O |
| ATOM | 5568 | N | ILE | 254 | 98.522 | 61.516 | 20.252 | 1.00 | 29.50 | B | N |
| ATOM | 5569 | CA | ILE | 254 | 97.692 | 60.403 | 20.701 | 1.00 | 26.40 | B | C |
| ATOM | 5570 | CB | ILE | 254 | 96.820 | 60.777 | 21.925 | 1.00 | 25.01 | B | C |
| ATOM | 5571 | CG2 | ILE | 254 | 96.017 | 59.564 | 22.369 | 1.00 | 21.48 | B | C |
| ATOM | 5572 | CG1 | ILE | 254 | 97.697 | 61.256 | 23.089 | 1.00 | 23.59 | B | C |
| ATOM | 5573 | CD1 | ILE | 254 | 98.231 | 62.661 | 22.921 | 1.00 | 23.22 | B | C |
| ATOM | 5574 | C | ILE | 254 | 96.757 | 59.905 | 19.611 | 1.00 | 24.49 | B | C |
| ATOM | 5575 | O | ILE | 254 | 96.163 | 60.692 | 18.876 | 1.00 | 26.36 | B | O |
| ATOM | 5576 | N | VAL | 255 | 96.628 | 58.587 | 19.516 | 1.00 | 26.63 | B | N |
| ATOM | 5577 | CA | VAL | 255 | 95.758 | 57.981 | 18.521 | 1.00 | 25.37 | B | C |
| ATOM | 5578 | CB | VAL | 255 | 96.553 | 57.259 | 17.428 | 1.00 | 15.78 | B | C |
| ATOM | 5579 | CG1 | VAL | 255 | 95.672 | 57.064 | 16.198 | 1.00 | 14.23 | B | C |
| ATOM | 5580 | CG2 | VAL | 255 | 97.805 | 58.036 | 17.089 | 1.00 | 16.42 | B | C |
| ATOM | 5581 | C | VAL | 255 | 94.907 | 56.947 | 19.221 | 1.00 | 23.12 | B | C |
| ATOM | 5582 | O | VAL | 255 | 95.444 | 56.089 | 19.916 | 1.00 | 25.12 | B | O |
| ATOM | 5583 | N | THR | 256 | 93.591 | 57.012 | 19.036 | 1.00 | 8.41 | B | N |
| ATOM | 5584 | CA | THR | 256 | 92.709 | 56.052 | 19.689 | 1.00 | 8.83 | B | C |
| ATOM | 5585 | CB | THR | 256 | 92.529 | 56.416 | 21.189 | 1.00 | 19.33 | B | C |
| ATOM | 5586 | OG1 | THR | 256 | 91.459 | 55.645 | 21.755 | 1.00 | 15.37 | B | O |
| ATOM | 5587 | CG2 | THR | 256 | 92.255 | 57.908 | 21.344 | 1.00 | 18.18 | B | C |
| ATOM | 5588 | C | THR | 256 | 91.353 | 55.955 | 18.992 | 1.00 | 12.31 | B | C |
| ATOM | 5589 | O | THR | 256 | 90.941 | 56.881 | 18.308 | 1.00 | 8.47 | B | O |
| ATOM | 5590 | N | ASP | 257 | 90.673 | 54.824 | 19.162 | 1.00 | 17.26 | B | N |
| ATOM | 5591 | CA | ASP | 257 | 89.375 | 54.601 | 18.530 | 1.00 | 17.64 | B | C |
| ATOM | 5592 | CB | ASP | 257 | 89.491 | 53.474 | 17.491 | 1.00 | 29.20 | B | C |
| ATOM | 5593 | CG | ASP | 257 | 89.534 | 52.074 | 18.122 | 1.00 | 34.56 | B | C |
| ATOM | 5594 | OD1 | ASP | 257 | 89.894 | 51.957 | 19.313 | 1.00 | 35.03 | B | O |
| ATOM | 5595 | OD2 | ASP | 257 | 89.220 | 51.084 | 17.421 | 1.00 | 39.83 | B | O |
| ATOM | 5596 | C | ASP | 257 | 88.267 | 54.259 | 19.535 | 1.00 | 14.23 | B | C |
| ATOM | 5597 | O | ASP | 257 | 87.243 | 53.660 | 19.169 | 1.00 | 13.47 | B | O |
| ATOM | 5598 | N | GLY | 258 | 88.462 | 54.634 | 20.798 | 1.00 | 26.33 | B | N |
| ATOM | 5599 | CA | GLY | 258 | 87.450 | 54.331 | 21.793 | 1.00 | 28.75 | B | C |
| ATOM | 5600 | C | GLY | 258 | 87.546 | 55.109 | 23.088 | 1.00 | 32.57 | B | C |
| ATOM | 5601 | O | GLY | 258 | 88.615 | 55.601 | 23.476 | 1.00 | 28.29 | B | O |
| ATOM | 5602 | N | GLU | 259 | 86.404 | 55.231 | 23.755 | 1.00 | 39.52 | B | N |
| ATOM | 5603 | CA | GLU | 259 | 86.335 | 55.931 | 25.025 | 1.00 | 41.40 | B | C |
| ATOM | 5604 | CB | GLU | 259 | 84.905 | 55.925 | 25.555 | 1.00 | 36.52 | B | C |
| ATOM | 5605 | CG | GLU | 259 | 83.950 | 56.783 | 24.749 | 1.00 | 44.30 | B | C |
| ATOM | 5606 | CD | GLU | 259 | 82.509 | 56.415 | 24.994 | 1.00 | 48.11 | B | C |
| ATOM | 5607 | OE1 | GLU | 259 | 81.625 | 57.175 | 24.546 | 1.00 | 54.86 | B | O |
| ATOM | 5608 | OE2 | GLU | 259 | 82.262 | 55.360 | 25.626 | 1.00 | 48.13 | B | O |
| ATOM | 5609 | C | GLU | 259 | 87.240 | 55.210 | 26.003 | 1.00 | 40.26 | B | C |
| ATOM | 5610 | O | GLU | 259 | 87.125 | 53.999 | 26.194 | 1.00 | 37.43 | B | O |
| ATOM | 5611 | N | SER | 260 | 88.155 | 55.953 | 26.610 | 1.00 | 34.06 | B | N |
| ATOM | 5612 | CA | SER | 260 | 89.067 | 55.369 | 27.576 | 1.00 | 37.22 | B | C |
| ATOM | 5613 | CB | SER | 260 | 90.041 | 56.432 | 28.083 | 1.00 | 50.00 | B | C |
| ATOM | 5614 | OG | SER | 260 | 89.341 | 57.516 | 28.666 | 1.00 | 50.51 | B | O |
| ATOM | 5615 | C | SER | 260 | 88.261 | 54.814 | 28.740 | 1.00 | 37.12 | B | C |
| ATOM | 5616 | O | SER | 260 | 87.177 | 55.300 | 29.043 | 1.00 | 33.15 | B | O |
| ATOM | 5617 | N | HIS | 261 | 88.781 | 53.787 | 29.392 | 1.00 | 36.47 | B | N |
| ATOM | 5618 | CA | HIS | 261 | 88.084 | 53.212 | 30.527 | 1.00 | 40.82 | B | C |
| ATOM | 5619 | CB | HIS | 261 | 88.509 | 51.755 | 30.728 | 1.00 | 21.13 | B | C |
| ATOM | 5620 | CG | HIS | 261 | 87.908 | 50.809 | 29.732 | 1.00 | 24.33 | B | C |
| ATOM | 5621 | CD2 | HIS | 261 | 88.345 | 50.398 | 28.519 | 1.00 | 23.44 | B | C |

Fig. 19: A-78

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 5622 | ND1 | HIS | 261 | 86.688 | 50.197 | 29.925 | 1.00 | 25.81 | B | N |
| ATOM | 5623 | CE1 | HIS | 261 | 86.400 | 49.448 | 28.876 | 1.00 | 25.88 | B | C |
| ATOM | 5624 | NE2 | HIS | 261 | 87.390 | 49.554 | 28.009 | 1.00 | 23.15 | B | N |
| ATOM | 5625 | C | HIS | 261 | 88.394 | 54.045 | 31.761 | 1.00 | 41.88 | B | C |
| ATOM | 5626 | O | HIS | 261 | 87.711 | 53.940 | 32.779 | 1.00 | 39.10 | B | O |
| ATOM | 5627 | N | ASP | 262 | 89.425 | 54.880 | 31.657 | 1.00 | 49.36 | B | N |
| ATOM | 5628 | CA | ASP | 262 | 89.825 | 55.758 | 32.753 | 1.00 | 54.33 | B | C |
| ATOM | 5629 | CB | ASP | 262 | 91.343 | 55.676 | 32.985 | 1.00 | 33.92 | B | C |
| ATOM | 5630 | CG | ASP | 262 | 92.124 | 55.281 | 31.733 | 1.00 | 33.92 | B | C |
| ATOM | 5631 | OD1 | ASP | 262 | 91.724 | 55.659 | 30.611 | 1.00 | 33.92 | B | O |
| ATOM | 5632 | OD2 | ASP | 262 | 93.162 | 54.600 | 31.875 | 1.00 | 33.92 | B | O |
| ATOM | 5633 | C | ASP | 262 | 89.418 | 57.218 | 32.507 | 1.00 | 54.38 | B | C |
| ATOM | 5634 | O | ASP | 262 | 90.221 | 58.134 | 32.700 | 1.00 | 54.24 | B | O |
| ATOM | 5635 | N | ASN | 263 | 88.171 | 57.424 | 32.085 | 1.00 | 68.10 | B | N |
| ATOM | 5636 | CA | ASN | 263 | 87.646 | 58.765 | 31.813 | 1.00 | 69.27 | B | C |
| ATOM | 5637 | CB | ASN | 263 | 86.123 | 58.734 | 31.630 | 1.00 | 82.52 | B | C |
| ATOM | 5638 | CG | ASN | 263 | 85.660 | 57.631 | 30.707 | 1.00 | 86.89 | B | C |
| ATOM | 5639 | OD1 | ASN | 263 | 85.981 | 57.626 | 29.519 | 1.00 | 88.39 | B | O |
| ATOM | 5640 | ND2 | ASN | 263 | 84.893 | 56.686 | 31.249 | 1.00 | 81.39 | B | N |
| ATOM | 5641 | C | ASN | 263 | 87.948 | 59.670 | 32.998 | 1.00 | 69.91 | B | C |
| ATOM | 5642 | O | ASN | 263 | 88.360 | 60.822 | 32.841 | 1.00 | 68.81 | B | O |
| ATOM | 5643 | N | TYR | 264 | 87.732 | 59.122 | 34.187 | 1.00 | 59.82 | B | N |
| ATOM | 5644 | CA | TYR | 264 | 87.925 | 59.837 | 35.432 | 1.00 | 57.67 | B | C |
| ATOM | 5645 | CB | TYR | 264 | 87.914 | 58.853 | 36.590 | 1.00 | 108.49 | B | C |
| ATOM | 5646 | CG | TYR | 264 | 86.626 | 58.083 | 36.660 | 1.00 | 108.49 | B | C |
| ATOM | 5647 | CD1 | TYR | 264 | 86.284 | 57.171 | 35.663 | 1.00 | 108.49 | B | C |
| ATOM | 5648 | CE1 | TYR | 264 | 85.074 | 56.490 | 35.698 | 1.00 | 108.49 | B | C |
| ATOM | 5649 | CD2 | TYR | 264 | 85.723 | 58.292 | 37.699 | 1.00 | 108.49 | B | C |
| ATOM | 5650 | CE2 | TYR | 264 | 84.509 | 57.615 | 37.744 | 1.00 | 108.49 | B | C |
| ATOM | 5651 | CZ | TYR | 264 | 84.190 | 56.717 | 36.741 | 1.00 | 108.49 | B | C |
| ATOM | 5652 | OH | TYR | 264 | 82.987 | 56.052 | 36.783 | 1.00 | 108.49 | B | O |
| ATOM | 5653 | C | TYR | 264 | 89.156 | 60.710 | 35.512 | 1.00 | 56.32 | B | C |
| ATOM | 5654 | O | TYR | 264 | 89.047 | 61.935 | 35.549 | 1.00 | 53.45 | B | O |
| ATOM | 5655 | N | ARG | 265 | 90.331 | 60.098 | 35.527 | 1.00 | 41.74 | B | N |
| ATOM | 5656 | CA | ARG | 265 | 91.544 | 60.892 | 35.641 | 1.00 | 40.64 | B | C |
| ATOM | 5657 | CB | ARG | 265 | 92.610 | 60.127 | 36.427 | 1.00 | 58.89 | B | C |
| ATOM | 5658 | CG | ARG | 265 | 93.152 | 58.875 | 35.779 | 1.00 | 59.34 | B | C |
| ATOM | 5659 | CD | ARG | 265 | 94.501 | 58.614 | 36.400 | 1.00 | 61.17 | B | C |
| ATOM | 5660 | NE | ARG | 265 | 95.183 | 57.456 | 35.851 | 1.00 | 66.56 | B | N |
| ATOM | 5661 | CZ | ARG | 265 | 96.506 | 57.349 | 35.784 | 1.00 | 66.73 | B | C |
| ATOM | 5662 | NH1 | ARG | 265 | 97.281 | 58.334 | 36.227 | 1.00 | 71.36 | B | N |
| ATOM | 5663 | NH2 | ARG | 265 | 97.059 | 56.256 | 35.280 | 1.00 | 70.70 | B | N |
| ATOM | 5664 | C | ARG | 265 | 92.147 | 61.423 | 34.347 | 1.00 | 39.89 | B | C |
| ATOM | 5665 | O | ARG | 265 | 93.311 | 61.833 | 34.319 | 1.00 | 41.20 | B | O |
| ATOM | 5666 | N | LEU | 266 | 91.360 | 61.433 | 33.278 | 1.00 | 45.12 | B | N |
| ATOM | 5667 | CA | LEU | 266 | 91.855 | 61.947 | 32.007 | 1.00 | 46.69 | B | C |
| ATOM | 5668 | CB | LEU | 266 | 90.885 | 61.580 | 30.886 | 1.00 | 30.69 | B | C |
| ATOM | 5669 | CG | LEU | 266 | 91.357 | 61.919 | 29.480 | 1.00 | 29.90 | B | C |
| ATOM | 5670 | CD1 | LEU | 266 | 92.760 | 61.369 | 29.232 | 1.00 | 32.24 | B | C |
| ATOM | 5671 | CD2 | LEU | 266 | 90.347 | 61.344 | 28.500 | 1.00 | 26.36 | B | C |
| ATOM | 5672 | C | LEU | 266 | 91.989 | 63.466 | 32.139 | 1.00 | 49.51 | B | C |
| ATOM | 5673 | O | LEU | 266 | 92.861 | 64.093 | 31.541 | 1.00 | 49.39 | B | O |
| ATOM | 5674 | N | LYS | 267 | 91.107 | 64.041 | 32.945 | 1.00 | 50.12 | B | N |
| ATOM | 5675 | CA | LYS | 267 | 91.097 | 65.473 | 33.206 | 1.00 | 52.43 | B | C |
| ATOM | 5676 | CB | LYS | 267 | 89.927 | 65.807 | 34.136 | 1.00 | 99.33 | B | C |
| ATOM | 5677 | CG | LYS | 267 | 89.719 | 67.279 | 34.431 | 1.00 | 99.33 | B | C |
| ATOM | 5678 | CD | LYS | 267 | 88.623 | 67.863 | 33.558 | 1.00 | 99.33 | B | C |
| ATOM | 5679 | CE | LYS | 267 | 88.211 | 69.242 | 34.049 | 1.00 | 99.33 | B | C |
| ATOM | 5680 | NZ | LYS | 267 | 87.044 | 69.788 | 33.293 | 1.00 | 99.33 | B | N |
| ATOM | 5681 | C | LYS | 267 | 92.417 | 65.835 | 33.882 | 1.00 | 51.92 | B | C |
| ATOM | 5682 | O | LYS | 267 | 93.126 | 66.738 | 33.440 | 1.00 | 51.44 | B | O |
| ATOM | 5683 | N | GLN | 268 | 92.736 | 65.115 | 34.956 | 1.00 | 36.69 | B | N |
| ATOM | 5684 | CA | GLN | 268 | 93.968 | 65.338 | 35.709 | 1.00 | 35.66 | B | C |
| ATOM | 5685 | CB | GLN | 268 | 94.098 | 64.324 | 36.841 | 1.00 | 127.61 | B | C |
| ATOM | 5686 | CG | GLN | 268 | 93.032 | 64.387 | 37.906 | 1.00 | 127.61 | B | C |
| ATOM | 5687 | CD | GLN | 268 | 93.203 | 63.286 | 38.941 | 1.00 | 127.61 | B | C |
| ATOM | 5688 | OE1 | GLN | 268 | 92.487 | 63.236 | 39.939 | 1.00 | 127.61 | B | O |
| ATOM | 5689 | NE2 | GLN | 268 | 94.158 | 62.392 | 38.702 | 1.00 | 127.61 | B | N |
| ATOM | 5690 | C | GLN | 268 | 95.203 | 65.210 | 34.824 | 1.00 | 31.41 | B | C |
| ATOM | 5691 | O | GLN | 268 | 96.044 | 66.108 | 34.788 | 1.00 | 32.59 | B | O |
| ATOM | 5692 | N | VAL | 269 | 95.308 | 64.085 | 34.114 | 1.00 | 29.89 | B | N |
| ATOM | 5693 | CA | VAL | 269 | 96.457 | 63.831 | 33.256 | 1.00 | 27.64 | B | C |
| ATOM | 5694 | CB | VAL | 269 | 96.321 | 62.467 | 32.516 | 1.00 | 26.10 | B | C |

Fig. 19: A-79

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 5695 | CG1 | VAL | 269 | 97.551 | 62.215 | 31.663 | 1.00 | 21.75 | B | C |
| ATOM | 5696 | CG2 | VAL | 269 | 96.161 | 61.338 | 33.520 | 1.00 | 23.96 | B | C |
| ATOM | 5697 | C | VAL | 269 | 96.683 | 64.956 | 32.246 | 1.00 | 27.23 | B | C |
| ATOM | 5698 | O | VAL | 269 | 97.784 | 65.502 | 32.174 | 1.00 | 30.07 | B | O |
| ATOM | 5699 | N | ILE | 270 | 95.658 | 65.306 | 31.471 | 1.00 | 16.50 | B | N |
| ATOM | 5700 | CA | ILE | 270 | 95.797 | 66.379 | 30.487 | 1.00 | 17.12 | B | C |
| ATOM | 5701 | CB | ILE | 270 | 94.459 | 66.696 | 29.777 | 1.00 | 35.19 | B | C |
| ATOM | 5702 | CG2 | ILE | 270 | 94.594 | 67.973 | 28.937 | 1.00 | 29.81 | B | C |
| ATOM | 5703 | CG1 | ILE | 270 | 94.060 | 65.520 | 28.885 | 1.00 | 32.75 | B | C |
| ATOM | 5704 | CD1 | ILE | 270 | 95.062 | 65.231 | 27.778 | 1.00 | 33.87 | B | C |
| ATOM | 5705 | C | ILE | 270 | 96.275 | 67.631 | 31.210 | 1.00 | 20.99 | B | C |
| ATOM | 5706 | O | ILE | 270 | 97.060 | 68.413 | 30.670 | 1.00 | 19.77 | B | O |
| ATOM | 5707 | N | GLN | 271 | 95.802 | 67.796 | 32.444 | 1.00 | 57.05 | B | N |
| ATOM | 5708 | CA | GLN | 271 | 96.169 | 68.935 | 33.269 | 1.00 | 59.11 | B | C |
| ATOM | 5709 | CB | GLN | 271 | 95.440 | 68.865 | 34.610 | 1.00 | 85.78 | B | C |
| ATOM | 5710 | CG | GLN | 271 | 95.525 | 70.134 | 35.439 | 1.00 | 87.68 | B | C |
| ATOM | 5711 | CD | GLN | 271 | 94.967 | 71.338 | 34.708 | 1.00 | 90.18 | B | C |
| ATOM | 5712 | OE1 | GLN | 271 | 95.614 | 71.898 | 33.822 | 1.00 | 90.51 | B | O |
| ATOM | 5713 | NE2 | GLN | 271 | 93.752 | 71.735 | 35.065 | 1.00 | 91.75 | B | N |
| ATOM | 5714 | C | GLN | 271 | 97.673 | 68.932 | 33.495 | 1.00 | 61.57 | B | C |
| ATOM | 5715 | O | GLN | 271 | 98.359 | 69.896 | 33.172 | 1.00 | 64.26 | B | O |
| ATOM | 5716 | N | ASP | 272 | 98.184 | 67.837 | 34.042 | 1.00 | 39.03 | B | N |
| ATOM | 5717 | CA | ASP | 272 | 99.612 | 67.716 | 34.304 | 1.00 | 40.31 | B | C |
| ATOM | 5718 | CB | ASP | 272 | 99.922 | 66.338 | 34.890 | 1.00 | 54.12 | B | C |
| ATOM | 5719 | CG | ASP | 272 | 99.275 | 66.122 | 36.255 | 1.00 | 55.74 | B | C |
| ATOM | 5720 | OD1 | ASP | 272 | 99.087 | 64.949 | 36.647 | 1.00 | 57.81 | B | O |
| ATOM | 5721 | OD2 | ASP | 272 | 98.961 | 67.123 | 36.939 | 1.00 | 62.00 | B | O |
| ATOM | 5722 | C | ASP | 272 | 100.420 | 67.937 | 33.033 | 1.00 | 41.11 | B | C |
| ATOM | 5723 | O | ASP | 272 | 101.550 | 68.418 | 33.083 | 1.00 | 38.56 | B | O |
| ATOM | 5724 | N | CYS | 273 | 99.843 | 67.587 | 31.891 | 1.00 | 49.56 | B | N |
| ATOM | 5725 | CA | CYS | 273 | 100.538 | 67.776 | 30.629 | 1.00 | 47.99 | B | C |
| ATOM | 5726 | CB | CYS | 273 | 99.824 | 67.028 | 29.503 | 1.00 | 39.07 | B | C |
| ATOM | 5727 | SG | CYS | 273 | 100.050 | 65.235 | 29.538 | 1.00 | 37.17 | B | S |
| ATOM | 5728 | C | CYS | 273 | 100.628 | 69.257 | 30.291 | 1.00 | 48.36 | B | C |
| ATOM | 5729 | O | CYS | 273 | 101.602 | 69.695 | 29.686 | 1.00 | 42.67 | B | O |
| ATOM | 5730 | N | GLU | 274 | 99.609 | 70.022 | 30.682 | 1.00 | 40.12 | B | N |
| ATOM | 5731 | CA | GLU | 274 | 99.584 | 71.467 | 30.425 | 1.00 | 42.92 | B | C |
| ATOM | 5732 | CB | GLU | 274 | 98.187 | 72.055 | 30.703 | 1.00 | 40.77 | B | C |
| ATOM | 5733 | CG | GLU | 274 | 97.285 | 72.151 | 29.470 | 1.00 | 45.89 | B | C |
| ATOM | 5734 | CD | GLU | 274 | 97.830 | 73.108 | 28.405 | 1.00 | 51.00 | B | C |
| ATOM | 5735 | OE1 | GLU | 274 | 97.269 | 73.155 | 27.284 | 1.00 | 52.87 | B | O |
| ATOM | 5736 | OE2 | GLU | 274 | 98.816 | 73.818 | 28.691 | 1.00 | 55.56 | B | O |
| ATOM | 5737 | C | GLU | 274 | 100.615 | 72.172 | 31.293 | 1.00 | 45.34 | B | C |
| ATOM | 5738 | O | GLU | 274 | 101.309 | 73.081 | 30.842 | 1.00 | 47.54 | B | O |
| ATOM | 5739 | N | ASP | 275 | 100.711 | 71.735 | 32.542 | 1.00 | 77.40 | B | N |
| ATOM | 5740 | CA | ASP | 275 | 101.656 | 72.302 | 33.495 | 1.00 | 76.14 | B | C |
| ATOM | 5741 | CB | ASP | 275 | 101.456 | 71.665 | 34.871 | 1.00 | 72.98 | B | C |
| ATOM | 5742 | CG | ASP | 275 | 100.070 | 71.900 | 35.432 | 1.00 | 74.25 | B | C |
| ATOM | 5743 | OD1 | ASP | 275 | 99.160 | 72.258 | 34.656 | 1.00 | 77.95 | B | O |
| ATOM | 5744 | OD2 | ASP | 275 | 99.887 | 71.712 | 36.652 | 1.00 | 75.91 | B | O |
| ATOM | 5745 | C | ASP | 275 | 103.093 | 72.050 | 33.046 | 1.00 | 75.13 | B | C |
| ATOM | 5746 | O | ASP | 275 | 104.021 | 72.707 | 33.512 | 1.00 | 70.68 | B | O |
| ATOM | 5747 | N | GLU | 276 | 103.275 | 71.091 | 32.146 | 1.00 | 44.46 | B | N |
| ATOM | 5748 | CA | GLU | 276 | 104.606 | 70.757 | 31.668 | 1.00 | 44.11 | B | C |
| ATOM | 5749 | CB | GLU | 276 | 104.846 | 69.258 | 31.847 | 1.00 | 54.99 | B | C |
| ATOM | 5750 | CG | GLU | 276 | 104.556 | 68.799 | 33.266 | 1.00 | 54.86 | B | C |
| ATOM | 5751 | CD | GLU | 276 | 105.018 | 67.383 | 33.547 | 1.00 | 55.96 | B | C |
| ATOM | 5752 | OE1 | GLU | 276 | 104.861 | 66.934 | 34.705 | 1.00 | 56.67 | B | O |
| ATOM | 5753 | OE2 | GLU | 276 | 105.538 | 66.724 | 32.616 | 1.00 | 52.90 | B | O |
| ATOM | 5754 | C | GLU | 276 | 104.843 | 71.175 | 30.222 | 1.00 | 42.94 | B | C |
| ATOM | 5755 | O | GLU | 276 | 105.823 | 70.759 | 29.597 | 1.00 | 44.05 | B | O |
| ATOM | 5756 | N | ASN | 277 | 103.938 | 71.997 | 29.700 | 1.00 | 43.81 | B | N |
| ATOM | 5757 | CA | ASN | 277 | 104.043 | 72.505 | 28.338 | 1.00 | 43.78 | B | C |
| ATOM | 5758 | CB | ASN | 277 | 105.229 | 73.464 | 28.233 | 1.00 | 55.27 | B | C |
| ATOM | 5759 | CG | ASN | 277 | 105.219 | 74.514 | 29.311 | 1.00 | 60.19 | B | C |
| ATOM | 5760 | OD1 | ASN | 277 | 104.288 | 75.315 | 29.403 | 1.00 | 60.01 | B | O |
| ATOM | 5761 | ND2 | ASN | 277 | 106.256 | 74.518 | 30.145 | 1.00 | 59.15 | B | N |
| ATOM | 5762 | C | ASN | 277 | 104.188 | 71.428 | 27.261 | 1.00 | 40.13 | B | C |
| ATOM | 5763 | O | ASN | 277 | 105.083 | 71.515 | 26.416 | 1.00 | 41.11 | B | O |
| ATOM | 5764 | N | ILE | 278 | 103.309 | 70.427 | 27.278 | 1.00 | 17.87 | B | N |
| ATOM | 5765 | CA | ILE | 278 | 103.366 | 69.361 | 26.289 | 1.00 | 18.32 | B | C |
| ATOM | 5766 | CB | ILE | 278 | 103.110 | 67.975 | 26.928 | 1.00 | 22.06 | B | C |
| ATOM | 5767 | CG2 | ILE | 278 | 103.120 | 66.897 | 25.854 | 1.00 | 23.45 | B | C |

Fig. 19: A-80

```
ATOM   5768  CG1 ILE   278     104.172  67.675  27.987  1.00  19.51      B    C
ATOM   5769  CD1 ILE   278     103.941  66.373  28.707  1.00  21.79      B    C
ATOM   5770  C   ILE   278     102.316  69.579  25.213  1.00  18.92      B    C
ATOM   5771  O   ILE   278     101.132  69.378  25.463  1.00  19.26      B    O
ATOM   5772  N   GLN   279     102.749  69.994  24.024  1.00  49.21      B    N
ATOM   5773  CA  GLN   279     101.831  70.198  22.908  1.00  48.81      B    C
ATOM   5774  CB  GLN   279     102.579  70.633  21.652  1.00  63.04      B    C
ATOM   5775  CG  GLN   279     103.187  71.998  21.752  1.00  68.82      B    C
ATOM   5776  CD  GLN   279     102.173  73.043  22.155  1.00  72.74      B    C
ATOM   5777  OE1 GLN   279     101.233  73.328  21.410  1.00  66.98      B    O
ATOM   5778  NE2 GLN   279     102.352  73.618  23.345  1.00  72.33      B    N
ATOM   5779  C   GLN   279     101.175  68.864  22.640  1.00  46.68      B    C
ATOM   5780  O   GLN   279     101.861  67.859  22.467  1.00  43.60      B    O
ATOM   5781  N   ARG   280      99.851  68.848  22.595  1.00  28.30      B    N
ATOM   5782  CA  ARG   280      99.138  67.605  22.363  1.00  29.82      B    C
ATOM   5783  CB  ARG   280      98.276  67.277  23.575  1.00  38.67      B    C
ATOM   5784  CG  ARG   280      99.036  67.225  24.874  1.00  37.30      B    C
ATOM   5785  CD  ARG   280      98.068  67.012  26.018  1.00  36.97      B    C
ATOM   5786  NE  ARG   280      97.070  68.075  26.073  1.00  34.02      B    N
ATOM   5787  CZ  ARG   280      97.288  69.298  26.557  1.00  37.93      B    C
ATOM   5788  NH1 ARG   280      98.483  69.627  27.041  1.00  40.85      B    N
ATOM   5789  NH2 ARG   280      96.307  70.192  26.554  1.00  42.87      B    N
ATOM   5790  C   ARG   280      98.264  67.579  21.111  1.00  29.48      B    C
ATOM   5791  O   ARG   280      97.406  68.437  20.912  1.00  29.21      B    O
ATOM   5792  N   PHE   281      98.501  66.582  20.266  1.00  31.71      B    N
ATOM   5793  CA  PHE   281      97.713  66.392  19.066  1.00  33.70      B    C
ATOM   5794  CB  PHE   281      98.594  66.335  17.826  1.00  18.70      B    C
ATOM   5795  CG  PHE   281      99.324  67.604  17.555  1.00  21.73      B    C
ATOM   5796  CD1 PHE   281     100.438  67.950  18.308  1.00  25.58      B    C
ATOM   5797  CD2 PHE   281      98.887  68.469  16.551  1.00  23.46      B    C
ATOM   5798  CE1 PHE   281     101.111  69.136  18.070  1.00  25.64      B    C
ATOM   5799  CE2 PHE   281      99.554  69.665  16.301  1.00  21.19      B    C
ATOM   5800  CZ  PHE   281     100.669  69.999  17.064  1.00  22.62      B    C
ATOM   5801  C   PHE   281      97.025  65.060  19.266  1.00  34.41      B    C
ATOM   5802  O   PHE   281      97.677  64.053  19.509  1.00  36.78      B    O
ATOM   5803  N   SER   282      95.704  65.061  19.202  1.00  16.00      B    N
ATOM   5804  CA  SER   282      94.962  63.835  19.374  1.00  17.85      B    C
ATOM   5805  CB  SER   282      93.973  63.973  20.528  1.00  14.79      B    C
ATOM   5806  OG  SER   282      93.036  64.997  20.286  1.00  11.34      B    O
ATOM   5807  C   SER   282      94.231  63.507  18.093  1.00  19.73      B    C
ATOM   5808  O   SER   282      93.909  64.389  17.306  1.00  23.59      B    O
ATOM   5809  N   ILE   283      93.986  62.224  17.881  1.00  19.27      B    N
ATOM   5810  CA  ILE   283      93.288  61.779  16.693  1.00  17.19      B    C
ATOM   5811  CB  ILE   283      94.245  61.146  15.697  1.00   9.92      B    C
ATOM   5812  CG2 ILE   283      93.501  60.806  14.425  1.00  10.73      B    C
ATOM   5813  CG1 ILE   283      95.377  62.118  15.383  1.00   6.39      B    C
ATOM   5814  CD1 ILE   283      96.630  61.446  14.894  1.00   9.95      B    C
ATOM   5815  C   ILE   283      92.278  60.748  17.127  1.00  16.26      B    C
ATOM   5816  O   ILE   283      92.574  59.886  17.947  1.00  16.12      B    O
ATOM   5817  N   ALA   284      91.078  60.836  16.584  1.00  18.66      B    N
ATOM   5818  CA  ALA   284      90.050  59.896  16.955  1.00  18.68      B    C
ATOM   5819  CB  ALA   284      88.903  60.627  17.622  1.00  45.12      B    C
ATOM   5820  C   ALA   284      89.542  59.107  15.759  1.00  16.81      B    C
ATOM   5821  O   ALA   284      89.045  59.681  14.792  1.00  15.47      B    O
ATOM   5822  N   ILE   285      89.691  57.788  15.826  1.00  23.61      B    N
ATOM   5823  CA  ILE   285      89.205  56.922  14.772  1.00  17.81      B    C
ATOM   5824  CB  ILE   285      89.960  55.564  14.741  1.00  12.20      B    C
ATOM   5825  CG2 ILE   285      89.210  54.576  13.862  1.00   7.02      B    C
ATOM   5826  CG1 ILE   285      91.380  55.738  14.204  1.00   7.53      B    C
ATOM   5827  CD1 ILE   285      92.342  56.334  15.179  1.00   8.67      B    C
ATOM   5828  C   ILE   285      87.745  56.678  15.148  1.00  21.13      B    C
ATOM   5829  O   ILE   285      87.466  56.108  16.201  1.00  22.87      B    O
ATOM   5830  N   LEU   286      86.820  57.112  14.297  1.00  18.22      B    N
ATOM   5831  CA  LEU   286      85.399  56.937  14.581  1.00  18.70      B    C
ATOM   5832  CB  LEU   286      84.615  58.129  14.039  1.00  27.86      B    C
ATOM   5833  CG  LEU   286      85.105  59.512  14.456  1.00  30.68      B    C
ATOM   5834  CD1 LEU   286      84.112  60.536  13.961  1.00  33.24      B    C
ATOM   5835  CD2 LEU   286      85.249  59.599  15.963  1.00  32.35      B    C
ATOM   5836  C   LEU   286      84.774  55.645  14.044  1.00  19.15      B    C
ATOM   5837  O   LEU   286      83.552  55.458  14.122  1.00  19.99      B    O
ATOM   5838  N   GLY   287      85.609  54.752  13.520  1.00  37.37      B    N
ATOM   5839  CA  GLY   287      85.115  53.501  12.967  1.00  36.15      B    C
ATOM   5840  C   GLY   287      84.059  52.745  13.760  1.00  33.73      B    C
```

Fig. 19: A-81

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 5841 | O | GLY | 287 | 82.899 | 52.681 | 13.367 | 1.00 | 37.83 | B | O |
| ATOM | 5842 | N | HIS | 288 | 84.464 | 52.162 | 14.878 | 1.00 | 34.79 | B | N |
| ATOM | 5843 | CA | HIS | 288 | 83.563 | 51.376 | 15.700 | 1.00 | 32.75 | B | C |
| ATOM | 5844 | CB | HIS | 288 | 84.272 | 51.016 | 16.996 | 1.00 | 68.63 | B | C |
| ATOM | 5845 | CG | HIS | 288 | 85.486 | 50.181 | 16.763 | 1.00 | 70.54 | B | C |
| ATOM | 5846 | CD2 | HIS | 288 | 85.781 | 48.912 | 17.123 | 1.00 | 66.91 | B | C |
| ATOM | 5847 | ND1 | HIS | 288 | 86.520 | 50.600 | 15.955 | 1.00 | 65.20 | B | N |
| ATOM | 5848 | CE1 | HIS | 288 | 87.397 | 49.623 | 15.821 | 1.00 | 65.56 | B | C |
| ATOM | 5849 | NE2 | HIS | 288 | 86.972 | 48.586 | 16.519 | 1.00 | 64.05 | B | N |
| ATOM | 5850 | C | HIS | 288 | 82.214 | 52.006 | 15.968 | 1.00 | 30.23 | B | C |
| ATOM | 5851 | O | HIS | 288 | 81.180 | 51.398 | 15.711 | 1.00 | 29.80 | B | O |
| ATOM | 5852 | N | TYR | 289 | 82.219 | 53.233 | 16.461 | 1.00 | 26.68 | B | N |
| ATOM | 5853 | CA | TYR | 289 | 80.982 | 53.912 | 16.754 | 1.00 | 27.59 | B | C |
| ATOM | 5854 | CB | TYR | 289 | 81.287 | 55.288 | 17.309 | 1.00 | 20.91 | B | C |
| ATOM | 5855 | CG | TYR | 289 | 81.803 | 55.203 | 18.717 | 1.00 | 23.71 | B | C |
| ATOM | 5856 | CD1 | TYR | 289 | 83.163 | 55.293 | 18.997 | 1.00 | 24.30 | B | C |
| ATOM | 5857 | CE1 | TYR | 289 | 83.633 | 55.127 | 20.281 | 1.00 | 27.49 | B | C |
| ATOM | 5858 | CD2 | TYR | 289 | 80.928 | 54.947 | 19.764 | 1.00 | 26.60 | B | C |
| ATOM | 5859 | CE2 | TYR | 289 | 81.381 | 54.776 | 21.047 | 1.00 | 21.41 | B | C |
| ATOM | 5860 | CZ | TYR | 289 | 82.733 | 54.866 | 21.303 | 1.00 | 23.14 | B | C |
| ATOM | 5861 | OH | TYR | 289 | 83.166 | 54.686 | 22.597 | 1.00 | 27.79 | B | O |
| ATOM | 5862 | C | TYR | 289 | 80.039 | 54.015 | 15.572 | 1.00 | 29.36 | B | C |
| ATOM | 5863 | O | TYR | 289 | 78.849 | 53.720 | 15.692 | 1.00 | 28.55 | B | O |
| ATOM | 5864 | N | ASN | 290 | 80.551 | 54.414 | 14.419 | 1.00 | 30.33 | B | N |
| ATOM | 5865 | CA | ASN | 290 | 79.681 | 54.538 | 13.264 | 1.00 | 29.82 | B | C |
| ATOM | 5866 | CB | ASN | 290 | 80.390 | 55.290 | 12.141 | 1.00 | 19.88 | B | C |
| ATOM | 5867 | CG | ASN | 290 | 80.582 | 56.750 | 12.466 | 1.00 | 23.09 | B | C |
| ATOM | 5868 | OD1 | ASN | 290 | 79.681 | 57.395 | 13.005 | 1.00 | 24.51 | B | O |
| ATOM | 5869 | ND2 | ASN | 290 | 81.748 | 57.286 | 12.133 | 1.00 | 26.61 | B | N |
| ATOM | 5870 | C | ASN | 290 | 79.142 | 53.214 | 12.746 | 1.00 | 28.65 | B | C |
| ATOM | 5871 | O | ASN | 290 | 78.008 | 53.153 | 12.264 | 1.00 | 35.25 | B | O |
| ATOM | 5872 | N | ARG | 291 | 79.944 | 52.155 | 12.842 | 1.00 | 46.80 | B | N |
| ATOM | 5873 | CA | ARG | 291 | 79.513 | 50.850 | 12.362 | 1.00 | 46.11 | B | C |
| ATOM | 5874 | CB | ARG | 291 | 80.694 | 49.867 | 12.337 | 1.00 | 45.84 | B | C |
| ATOM | 5875 | CG | ARG | 291 | 81.661 | 50.063 | 11.152 | 1.00 | 50.80 | B | C |
| ATOM | 5876 | CD | ARG | 291 | 82.722 | 48.943 | 11.054 | 1.00 | 54.88 | B | C |
| ATOM | 5877 | NE | ARG | 291 | 83.916 | 49.157 | 11.883 | 1.00 | 47.06 | B | N |
| ATOM | 5878 | CZ | ARG | 291 | 84.884 | 50.030 | 11.603 | 1.00 | 56.55 | B | C |
| ATOM | 5879 | NH1 | ARG | 291 | 84.813 | 50.787 | 10.515 | 1.00 | 55.39 | B | N |
| ATOM | 5880 | NH2 | ARG | 291 | 85.936 | 50.131 | 12.401 | 1.00 | 53.31 | B | N |
| ATOM | 5881 | C | ARG | 291 | 78.367 | 50.296 | 13.207 | 1.00 | 43.91 | B | C |
| ATOM | 5882 | O | ARG | 291 | 77.338 | 49.876 | 12.676 | 1.00 | 47.17 | B | O |
| ATOM | 5883 | N | GLY | 292 | 78.531 | 50.306 | 14.523 | 1.00 | 18.83 | B | N |
| ATOM | 5884 | CA | GLY | 292 | 77.476 | 49.795 | 15.374 | 1.00 | 19.08 | B | C |
| ATOM | 5885 | C | GLY | 292 | 76.427 | 50.857 | 15.628 | 1.00 | 26.45 | B | C |
| ATOM | 5886 | O | GLY | 292 | 75.874 | 50.947 | 16.722 | 1.00 | 32.58 | B | O |
| ATOM | 5887 | N | ASN | 293 | 76.151 | 51.664 | 14.610 | 1.00 | 32.56 | B | N |
| ATOM | 5888 | CA | ASN | 293 | 75.177 | 52.740 | 14.724 | 1.00 | 34.89 | B | C |
| ATOM | 5889 | CB | ASN | 293 | 73.785 | 52.239 | 14.339 | 1.00 | 18.98 | B | C |
| ATOM | 5890 | CG | ASN | 293 | 73.623 | 52.066 | 12.846 | 1.00 | 25.56 | B | C |
| ATOM | 5891 | OD1 | ASN | 293 | 74.249 | 52.776 | 12.063 | 1.00 | 27.19 | B | O |
| ATOM | 5892 | ND2 | ASN | 293 | 72.767 | 51.132 | 12.440 | 1.00 | 26.33 | B | N |
| ATOM | 5893 | C | ASN | 293 | 75.116 | 53.389 | 16.111 | 1.00 | 36.22 | B | C |
| ATOM | 5894 | O | ASN | 293 | 74.054 | 53.448 | 16.722 | 1.00 | 31.70 | B | O |
| ATOM | 5895 | N | LEU | 294 | 76.247 | 53.875 | 16.614 | 1.00 | 40.17 | B | N |
| ATOM | 5896 | CA | LEU | 294 | 76.260 | 54.525 | 17.921 | 1.00 | 39.32 | B | C |
| ATOM | 5897 | CB | LEU | 294 | 77.141 | 53.737 | 18.901 | 1.00 | 27.66 | B | C |
| ATOM | 5898 | CG | LEU | 294 | 76.633 | 52.343 | 19.291 | 1.00 | 26.48 | B | C |
| ATOM | 5899 | CD1 | LEU | 294 | 77.463 | 51.781 | 20.440 | 1.00 | 27.02 | B | C |
| ATOM | 5900 | CD2 | LEU | 294 | 75.175 | 52.437 | 19.714 | 1.00 | 27.39 | B | C |
| ATOM | 5901 | C | LEU | 294 | 76.730 | 55.985 | 17.823 | 1.00 | 41.69 | B | C |
| ATOM | 5902 | O | LEU | 294 | 77.579 | 56.314 | 16.984 | 1.00 | 40.35 | B | O |
| ATOM | 5903 | N | SER | 295 | 76.158 | 56.860 | 18.656 | 1.00 | 29.47 | B | N |
| ATOM | 5904 | CA | SER | 295 | 76.534 | 58.272 | 18.644 | 1.00 | 29.33 | B | C |
| ATOM | 5905 | CB | SER | 295 | 75.802 | 59.063 | 19.740 | 1.00 | 35.11 | B | C |
| ATOM | 5906 | OG | SER | 295 | 76.336 | 60.371 | 19.894 | 1.00 | 41.79 | B | O |
| ATOM | 5907 | C | SER | 295 | 78.022 | 58.329 | 18.890 | 1.00 | 25.45 | B | C |
| ATOM | 5908 | O | SER | 295 | 78.583 | 57.444 | 19.533 | 1.00 | 22.32 | B | O |
| ATOM | 5909 | N | THR | 296 | 78.661 | 59.379 | 18.401 | 1.00 | 28.05 | B | N |
| ATOM | 5910 | CA | THR | 296 | 80.096 | 59.500 | 18.559 | 1.00 | 28.09 | B | C |
| ATOM | 5911 | CB | THR | 296 | 80.786 | 59.452 | 17.191 | 1.00 | 44.94 | B | C |
| ATOM | 5912 | OG1 | THR | 296 | 80.305 | 60.534 | 16.383 | 1.00 | 50.00 | B | O |
| ATOM | 5913 | CG2 | THR | 296 | 80.485 | 58.150 | 16.487 | 1.00 | 44.81 | B | C |

Fig. 19: A-82

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 5914 | C | THR | 296 | 80.519 | 60.792 | 19.227 | 1.00 | 29.07 | B | C |
| ATOM | 5915 | O | THR | 296 | 81.695 | 60.971 | 19.535 | 1.00 | 27.88 | B | O |
| ATOM | 5916 | N | GLU | 297 | 79.581 | 61.705 | 19.451 | 1.00 | 50.64 | B | N |
| ATOM | 5917 | CA | GLU | 297 | 79.970 | 62.978 | 20.038 | 1.00 | 54.10 | B | C |
| ATOM | 5918 | CB | GLU | 297 | 78.781 | 63.943 | 20.111 | 1.00 | 93.12 | B | C |
| ATOM | 5919 | CG | GLU | 297 | 77.787 | 63.695 | 21.213 | 1.00 | 100.15 | B | C |
| ATOM | 5920 | CD | GLU | 297 | 77.036 | 64.960 | 21.569 | 1.00 | 101.40 | B | C |
| ATOM | 5921 | OE1 | GLU | 297 | 76.160 | 64.911 | 22.455 | 1.00 | 104.84 | B | O |
| ATOM | 5922 | OE2 | GLU | 297 | 77.333 | 66.010 | 20.964 | 1.00 | 102.89 | B | O |
| ATOM | 5923 | C | GLU | 297 | 80.639 | 62.849 | 21.399 | 1.00 | 52.14 | B | C |
| ATOM | 5924 | O | GLU | 297 | 81.715 | 63.406 | 21.612 | 1.00 | 51.64 | B | O |
| ATOM | 5925 | N | LYS | 298 | 80.029 | 62.104 | 22.315 | 1.00 | 35.40 | B | N |
| ATOM | 5926 | CA | LYS | 298 | 80.622 | 61.942 | 23.636 | 1.00 | 35.40 | B | C |
| ATOM | 5927 | CB | LYS | 298 | 79.837 | 60.916 | 24.443 | 1.00 | 37.32 | B | C |
| ATOM | 5928 | CG | LYS | 298 | 80.199 | 60.902 | 25.910 | 1.00 | 46.03 | B | C |
| ATOM | 5929 | CD | LYS | 298 | 79.201 | 60.085 | 26.727 | 1.00 | 47.75 | B | C |
| ATOM | 5930 | CE | LYS | 298 | 77.777 | 60.625 | 26.578 | 1.00 | 51.57 | B | C |
| ATOM | 5931 | NZ | LYS | 298 | 77.676 | 62.075 | 26.908 | 1.00 | 55.89 | B | N |
| ATOM | 5932 | C | LYS | 298 | 82.087 | 61.518 | 23.514 | 1.00 | 33.00 | B | C |
| ATOM | 5933 | O | LYS | 298 | 82.939 | 61.933 | 24.310 | 1.00 | 33.88 | B | O |
| ATOM | 5934 | N | PHE | 299 | 82.371 | 60.699 | 22.505 | 1.00 | 29.00 | B | N |
| ATOM | 5935 | CA | PHE | 299 | 83.729 | 60.226 | 22.244 | 1.00 | 27.24 | B | C |
| ATOM | 5936 | CB | PHE | 299 | 83.701 | 59.054 | 21.263 | 1.00 | 39.15 | B | C |
| ATOM | 5937 | CG | PHE | 299 | 85.065 | 58.571 | 20.851 | 1.00 | 31.59 | B | C |
| ATOM | 5938 | CD1 | PHE | 299 | 86.020 | 58.237 | 21.806 | 1.00 | 28.04 | B | C |
| ATOM | 5939 | CD2 | PHE | 299 | 85.396 | 58.435 | 19.505 | 1.00 | 29.32 | B | C |
| ATOM | 5940 | CE1 | PHE | 299 | 87.284 | 57.776 | 21.422 | 1.00 | 27.45 | B | C |
| ATOM | 5941 | CE2 | PHE | 299 | 86.667 | 57.970 | 19.119 | 1.00 | 23.73 | B | C |
| ATOM | 5942 | CZ | PHE | 299 | 87.603 | 57.643 | 20.078 | 1.00 | 22.24 | B | C |
| ATOM | 5943 | C | PHE | 299 | 84.562 | 61.361 | 21.662 | 1.00 | 27.59 | B | C |
| ATOM | 5944 | O | PHE | 299 | 85.625 | 61.702 | 22.183 | 1.00 | 23.40 | B | O |
| ATOM | 5945 | N | VAL | 300 | 84.077 | 61.946 | 20.576 | 1.00 | 13.78 | B | N |
| ATOM | 5946 | CA | VAL | 300 | 84.791 | 63.050 | 19.944 | 1.00 | 18.73 | B | C |
| ATOM | 5947 | CB | VAL | 300 | 83.954 | 63.701 | 18.822 | 1.00 | 24.12 | B | C |
| ATOM | 5948 | CG1 | VAL | 300 | 84.616 | 64.979 | 18.363 | 1.00 | 27.69 | B | C |
| ATOM | 5949 | CG2 | VAL | 300 | 83.814 | 62.731 | 17.646 | 1.00 | 28.13 | B | C |
| ATOM | 5950 | C | VAL | 300 | 85.142 | 64.119 | 20.966 | 1.00 | 17.37 | B | C |
| ATOM | 5951 | O | VAL | 300 | 86.209 | 64.715 | 20.906 | 1.00 | 17.87 | B | O |
| ATOM | 5952 | N | GLU | 301 | 84.248 | 64.359 | 21.914 | 1.00 | 33.19 | B | N |
| ATOM | 5953 | CA | GLU | 301 | 84.520 | 65.377 | 22.915 | 1.00 | 33.85 | B | C |
| ATOM | 5954 | CB | GLU | 301 | 83.255 | 65.707 | 23.706 | 1.00 | 133.49 | B | C |
| ATOM | 5955 | CG | GLU | 301 | 83.426 | 66.851 | 24.703 | 1.00 | 135.76 | B | C |
| ATOM | 5956 | CD | GLU | 301 | 84.115 | 68.077 | 24.108 | 1.00 | 141.57 | B | C |
| ATOM | 5957 | OE1 | GLU | 301 | 83.669 | 68.566 | 23.046 | 1.00 | 141.12 | B | O |
| ATOM | 5958 | OE2 | GLU | 301 | 85.102 | 68.555 | 24.713 | 1.00 | 143.84 | B | O |
| ATOM | 5959 | C | GLU | 301 | 85.634 | 64.925 | 23.847 | 1.00 | 32.42 | B | C |
| ATOM | 5960 | O | GLU | 301 | 86.495 | 65.723 | 24.239 | 1.00 | 30.50 | B | O |
| ATOM | 5961 | N | GLU | 302 | 85.628 | 63.642 | 24.190 | 1.00 | 18.71 | B | N |
| ATOM | 5962 | CA | GLU | 302 | 86.663 | 63.091 | 25.060 | 1.00 | 18.52 | B | C |
| ATOM | 5963 | CB | GLU | 302 | 86.420 | 61.596 | 25.293 | 1.00 | 49.27 | B | C |
| ATOM | 5964 | CG | GLU | 302 | 87.438 | 60.934 | 26.207 | 1.00 | 49.02 | B | C |
| ATOM | 5965 | CD | GLU | 302 | 87.100 | 59.486 | 26.491 | 1.00 | 45.95 | B | C |
| ATOM | 5966 | OE1 | GLU | 302 | 86.051 | 59.237 | 27.118 | 1.00 | 45.93 | B | O |
| ATOM | 5967 | OE2 | GLU | 302 | 87.875 | 58.594 | 26.084 | 1.00 | 50.37 | B | O |
| ATOM | 5968 | C | GLU | 302 | 88.046 | 63.301 | 24.456 | 1.00 | 21.59 | B | C |
| ATOM | 5969 | O | GLU | 302 | 88.964 | 63.720 | 25.150 | 1.00 | 20.85 | B | O |
| ATOM | 5970 | N | ILE | 303 | 88.188 | 63.031 | 23.159 | 1.00 | 30.73 | B | N |
| ATOM | 5971 | CA | ILE | 303 | 89.479 | 63.175 | 22.472 | 1.00 | 30.78 | B | C |
| ATOM | 5972 | CB | ILE | 303 | 89.470 | 62.431 | 21.112 | 1.00 | 21.11 | B | C |
| ATOM | 5973 | CG2 | ILE | 303 | 90.865 | 62.406 | 20.518 | 1.00 | 16.29 | B | C |
| ATOM | 5974 | CG1 | ILE | 303 | 88.932 | 61.003 | 21.306 | 1.00 | 18.71 | B | C |
| ATOM | 5975 | CD1 | ILE | 303 | 89.501 | 60.262 | 22.515 | 1.00 | 15.17 | B | C |
| ATOM | 5976 | C | ILE | 303 | 89.922 | 64.625 | 22.242 | 1.00 | 32.81 | B | C |
| ATOM | 5977 | O | ILE | 303 | 91.097 | 64.955 | 22.415 | 1.00 | 35.30 | B | O |
| ATOM | 5978 | N | LYS | 304 | 88.989 | 65.485 | 21.847 | 1.00 | 41.13 | B | N |
| ATOM | 5979 | CA | LYS | 304 | 89.321 | 66.881 | 21.624 | 1.00 | 41.93 | B | C |
| ATOM | 5980 | CB | LYS | 304 | 88.087 | 67.695 | 21.239 | 1.00 | 34.23 | B | C |
| ATOM | 5981 | CG | LYS | 304 | 87.578 | 67.484 | 19.837 | 1.00 | 40.90 | B | C |
| ATOM | 5982 | CD | LYS | 304 | 86.491 | 68.498 | 19.526 | 1.00 | 42.43 | B | C |
| ATOM | 5983 | CE | LYS | 304 | 85.937 | 68.312 | 18.122 | 1.00 | 45.16 | B | C |
| ATOM | 5984 | NZ | LYS | 304 | 84.893 | 69.323 | 17.799 | 1.00 | 47.34 | B | N |
| ATOM | 5985 | C | LYS | 304 | 89.892 | 67.455 | 22.906 | 1.00 | 38.02 | B | C |
| ATOM | 5986 | O | LYS | 304 | 90.833 | 68.240 | 22.871 | 1.00 | 42.10 | B | O |

Fig. 19: A-83

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 5987 | N | SER | 305 | 89.322 | 67.066 | 24.043 | 1.00 | 21.53 | B | N |
| ATOM | 5988 | CA | SER | 305 | 89.788 | 67.571 | 25.335 | 1.00 | 18.69 | B | C |
| ATOM | 5989 | CB | SER | 305 | 88.872 | 67.096 | 26.460 | 1.00 | 39.18 | B | C |
| ATOM | 5990 | OG | SER | 305 | 89.039 | 65.715 | 26.696 | 1.00 | 35.86 | B | O |
| ATOM | 5991 | C | SER | 305 | 91.223 | 67.134 | 25.622 | 1.00 | 19.21 | B | C |
| ATOM | 5992 | O | SER | 305 | 91.935 | 67.754 | 26.418 | 1.00 | 21.78 | B | O |
| ATOM | 5993 | N | ILE | 306 | 91.652 | 66.063 | 24.969 | 1.00 | 47.39 | B | N |
| ATOM | 5994 | CA | ILE | 306 | 93.005 | 65.582 | 25.158 | 1.00 | 44.14 | B | C |
| ATOM | 5995 | CB | ILE | 306 | 93.129 | 64.131 | 24.682 | 1.00 | 20.56 | B | C |
| ATOM | 5996 | CG2 | ILE | 306 | 94.584 | 63.769 | 24.454 | 1.00 | 21.29 | B | C |
| ATOM | 5997 | CG1 | ILE | 306 | 92.479 | 63.210 | 25.713 | 1.00 | 23.19 | B | C |
| ATOM | 5998 | CD1 | ILE | 306 | 92.459 | 61.762 | 25.302 | 1.00 | 20.90 | B | C |
| ATOM | 5999 | C | ILE | 306 | 93.966 | 66.469 | 24.378 | 1.00 | 41.90 | B | C |
| ATOM | 6000 | O | ILE | 306 | 95.146 | 66.583 | 24.717 | 1.00 | 42.43 | B | O |
| ATOM | 6001 | N | ALA | 307 | 93.445 | 67.103 | 23.334 | 1.00 | 47.34 | B | N |
| ATOM | 6002 | CA | ALA | 307 | 94.247 | 67.979 | 22.497 | 1.00 | 49.53 | B | C |
| ATOM | 6003 | CB | ALA | 307 | 93.538 | 68.236 | 21.181 | 1.00 | 34.34 | B | C |
| ATOM | 6004 | C | ALA | 307 | 94.526 | 69.296 | 23.200 | 1.00 | 49.19 | B | C |
| ATOM | 6005 | O | ALA | 307 | 93.952 | 69.595 | 24.253 | 1.00 | 48.18 | B | O |
| ATOM | 6006 | N | SER | 308 | 95.415 | 70.078 | 22.604 | 1.00 | 31.36 | B | N |
| ATOM | 6007 | CA | SER | 308 | 95.801 | 71.367 | 23.141 | 1.00 | 34.29 | B | C |
| ATOM | 6008 | CB | SER | 308 | 97.299 | 71.580 | 22.943 | 1.00 | 9.08 | B | C |
| ATOM | 6009 | OG | SER | 308 | 98.040 | 70.819 | 23.867 | 1.00 | 12.47 | B | O |
| ATOM | 6010 | C | SER | 308 | 95.054 | 72.489 | 22.446 | 1.00 | 37.94 | B | C |
| ATOM | 6011 | O | SER | 308 | 94.703 | 72.373 | 21.272 | 1.00 | 35.28 | B | O |
| ATOM | 6012 | N | GLU | 309 | 94.813 | 73.575 | 23.178 | 1.00 | 31.30 | B | N |
| ATOM | 6013 | CA | GLU | 309 | 94.137 | 74.735 | 22.614 | 1.00 | 34.79 | B | C |
| ATOM | 6014 | CB | GLU | 309 | 93.786 | 75.736 | 23.721 | 1.00 | 74.37 | B | C |
| ATOM | 6015 | CG | GLU | 309 | 92.834 | 75.203 | 24.787 | 1.00 | 79.74 | B | C |
| ATOM | 6016 | CD | GLU | 309 | 91.461 | 74.845 | 24.234 | 1.00 | 82.50 | B | C |
| ATOM | 6017 | OE1 | GLU | 309 | 90.533 | 74.618 | 25.043 | 1.00 | 84.83 | B | O |
| ATOM | 6018 | OE2 | GLU | 309 | 91.307 | 74.784 | 22.995 | 1.00 | 86.65 | B | O |
| ATOM | 6019 | C | GLU | 309 | 95.138 | 75.359 | 21.642 | 1.00 | 35.54 | B | C |
| ATOM | 6020 | O | GLU | 309 | 96.321 | 75.480 | 21.971 | 1.00 | 37.19 | B | O |
| ATOM | 6021 | N | PRO | 310 | 94.685 | 75.762 | 20.435 | 1.00 | 19.46 | B | N |
| ATOM | 6022 | CD | PRO | 310 | 95.588 | 76.399 | 19.457 | 1.00 | 19.32 | B | C |
| ATOM | 6023 | CA | PRO | 310 | 93.324 | 75.694 | 19.890 | 1.00 | 19.65 | B | C |
| ATOM | 6024 | CB | PRO | 310 | 93.362 | 76.729 | 18.770 | 1.00 | 21.15 | B | C |
| ATOM | 6025 | CG | PRO | 310 | 94.715 | 76.515 | 18.203 | 1.00 | 20.71 | B | C |
| ATOM | 6026 | C | PRO | 310 | 92.884 | 74.312 | 19.384 | 1.00 | 20.14 | B | C |
| ATOM | 6027 | O | PRO | 310 | 93.368 | 73.816 | 18.374 | 1.00 | 16.93 | B | O |
| ATOM | 6028 | N | THR | 311 | 91.945 | 73.714 | 20.101 | 1.00 | 34.98 | B | N |
| ATOM | 6029 | CA | THR | 311 | 91.410 | 72.410 | 19.764 | 1.00 | 35.85 | B | C |
| ATOM | 6030 | CB | THR | 311 | 89.985 | 72.276 | 20.321 | 1.00 | 54.06 | B | C |
| ATOM | 6031 | OG1 | THR | 311 | 89.327 | 71.159 | 19.711 | 1.00 | 58.22 | B | O |
| ATOM | 6032 | CG2 | THR | 311 | 89.195 | 73.556 | 20.052 | 1.00 | 57.14 | B | C |
| ATOM | 6033 | C | THR | 311 | 91.390 | 72.103 | 18.265 | 1.00 | 37.72 | B | C |
| ATOM | 6034 | O | THR | 311 | 91.801 | 71.022 | 17.847 | 1.00 | 38.89 | B | O |
| ATOM | 6035 | N | GLU | 312 | 90.929 | 73.049 | 17.451 | 1.00 | 45.13 | B | N |
| ATOM | 6036 | CA | GLU | 312 | 90.842 | 72.825 | 16.004 | 1.00 | 43.75 | B | C |
| ATOM | 6037 | CB | GLU | 312 | 90.160 | 74.008 | 15.309 | 1.00 | 94.13 | B | C |
| ATOM | 6038 | CG | GLU | 312 | 90.848 | 75.342 | 15.528 | 1.00 | 95.89 | B | C |
| ATOM | 6039 | CD | GLU | 312 | 90.633 | 76.309 | 14.376 | 1.00 | 95.00 | B | C |
| ATOM | 6040 | OE1 | GLU | 312 | 90.998 | 77.496 | 14.516 | 1.00 | 98.35 | B | O |
| ATOM | 6041 | OE2 | GLU | 312 | 90.109 | 75.880 | 13.327 | 1.00 | 95.87 | B | O |
| ATOM | 6042 | C | GLU | 312 | 92.168 | 72.547 | 15.310 | 1.00 | 42.37 | B | C |
| ATOM | 6043 | O | GLU | 312 | 92.219 | 71.771 | 14.367 | 1.00 | 42.33 | B | O |
| ATOM | 6044 | N | LYS | 313 | 93.240 | 73.180 | 15.763 | 1.00 | 62.67 | B | N |
| ATOM | 6045 | CA | LYS | 313 | 94.537 | 72.966 | 15.141 | 1.00 | 61.87 | B | C |
| ATOM | 6046 | CB | LYS | 313 | 95.368 | 74.255 | 15.192 | 1.00 | 80.35 | B | C |
| ATOM | 6047 | CG | LYS | 313 | 94.954 | 75.308 | 14.167 | 1.00 | 80.23 | B | C |
| ATOM | 6048 | CD | LYS | 313 | 95.351 | 74.917 | 12.745 | 1.00 | 76.53 | B | C |
| ATOM | 6049 | CE | LYS | 313 | 96.790 | 75.307 | 12.430 | 1.00 | 78.57 | B | C |
| ATOM | 6050 | NZ | LYS | 313 | 97.781 | 74.730 | 13.383 | 1.00 | 83.05 | B | N |
| ATOM | 6051 | C | LYS | 313 | 95.308 | 71.832 | 15.800 | 1.00 | 63.02 | B | C |
| ATOM | 6052 | O | LYS | 313 | 96.473 | 71.610 | 15.491 | 1.00 | 65.34 | B | O |
| ATOM | 6053 | N | HIS | 314 | 94.656 | 71.103 | 16.697 | 1.00 | 42.28 | B | N |
| ATOM | 6054 | CA | HIS | 314 | 95.326 | 70.011 | 17.391 | 1.00 | 43.13 | B | C |
| ATOM | 6055 | CB | HIS | 314 | 95.631 | 70.426 | 18.828 | 1.00 | 51.27 | B | C |
| ATOM | 6056 | CG | HIS | 314 | 96.611 | 71.551 | 18.938 | 1.00 | 48.13 | B | C |
| ATOM | 6057 | CD2 | HIS | 314 | 96.423 | 72.880 | 19.111 | 1.00 | 47.60 | B | C |
| ATOM | 6058 | ND1 | HIS | 314 | 97.973 | 71.364 | 18.847 | 1.00 | 47.71 | B | N |
| ATOM | 6059 | CE1 | HIS | 314 | 98.582 | 72.530 | 18.960 | 1.00 | 47.00 | B | C |

Fig. 19: A-84

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 6060 | NE2 | HIS | 314 | 97.664 | 73.466 | 19.121 | 1.00 | 47.39 | B | N |
| ATOM | 6061 | C | HIS | 314 | 94.540 | 68.706 | 17.405 | 1.00 | 43.26 | B | C |
| ATOM | 6062 | O | HIS | 314 | 95.034 | 67.690 | 17.896 | 1.00 | 46.66 | B | O |
| ATOM | 6063 | N | PHE | 315 | 93.324 | 68.732 | 16.868 | 1.00 | 55.79 | B | N |
| ATOM | 6064 | CA | PHE | 315 | 92.475 | 67.546 | 16.835 | 1.00 | 55.59 | B | C |
| ATOM | 6065 | CB | PHE | 315 | 91.175 | 67.834 | 17.578 | 1.00 | 29.85 | B | C |
| ATOM | 6066 | CG | PHE | 315 | 90.175 | 66.731 | 17.499 | 1.00 | 24.83 | B | C |
| ATOM | 6067 | CD1 | PHE | 315 | 90.445 | 65.490 | 18.057 | 1.00 | 26.67 | B | C |
| ATOM | 6068 | CD2 | PHE | 315 | 88.944 | 66.942 | 16.890 | 1.00 | 22.91 | B | C |
| ATOM | 6069 | CE1 | PHE | 315 | 89.503 | 64.473 | 18.016 | 1.00 | 21.62 | B | C |
| ATOM | 6070 | CE2 | PHE | 315 | 87.989 | 65.939 | 16.838 | 1.00 | 23.61 | B | C |
| ATOM | 6071 | CZ | PHE | 315 | 88.268 | 64.700 | 17.404 | 1.00 | 25.28 | B | C |
| ATOM | 6072 | C | PHE | 315 | 92.172 | 67.086 | 15.412 | 1.00 | 56.31 | B | C |
| ATOM | 6073 | O | PHE | 315 | 91.948 | 67.903 | 14.516 | 1.00 | 57.71 | B | O |
| ATOM | 6074 | N | PHE | 316 | 92.170 | 65.772 | 15.212 | 1.00 | 44.89 | B | N |
| ATOM | 6075 | CA | PHE | 316 | 91.898 | 65.200 | 13.899 | 1.00 | 41.94 | B | C |
| ATOM | 6076 | CB | PHE | 316 | 93.175 | 64.621 | 13.282 | 1.00 | 20.23 | B | C |
| ATOM | 6077 | CG | PHE | 316 | 94.195 | 65.652 | 12.900 | 1.00 | 23.85 | B | C |
| ATOM | 6078 | CD1 | PHE | 316 | 95.118 | 66.114 | 13.828 | 1.00 | 19.44 | B | C |
| ATOM | 6079 | CD2 | PHE | 316 | 94.229 | 66.165 | 11.605 | 1.00 | 20.70 | B | C |
| ATOM | 6080 | CE1 | PHE | 316 | 96.066 | 67.074 | 13.475 | 1.00 | 22.01 | B | C |
| ATOM | 6081 | CE2 | PHE | 316 | 95.171 | 67.125 | 11.242 | 1.00 | 23.81 | B | C |
| ATOM | 6082 | CZ | PHE | 316 | 96.092 | 67.580 | 12.180 | 1.00 | 24.04 | B | C |
| ATOM | 6083 | C | PHE | 316 | 90.841 | 64.107 | 13.990 | 1.00 | 39.87 | B | C |
| ATOM | 6084 | O | PHE | 316 | 90.845 | 63.302 | 14.910 | 1.00 | 39.11 | B | O |
| ATOM | 6085 | N | ASN | 317 | 89.938 | 64.088 | 13.020 | 1.00 | 36.72 | B | N |
| ATOM | 6086 | CA | ASN | 317 | 88.863 | 63.110 | 12.978 | 1.00 | 37.94 | B | C |
| ATOM | 6087 | CB | ASN | 317 | 87.538 | 63.826 | 12.746 | 1.00 | 58.19 | B | C |
| ATOM | 6088 | CG | ASN | 317 | 86.496 | 63.443 | 13.752 | 1.00 | 61.18 | B | C |
| ATOM | 6089 | OD1 | ASN | 317 | 86.408 | 62.284 | 14.144 | 1.00 | 63.11 | B | O |
| ATOM | 6090 | ND2 | ASN | 317 | 85.688 | 64.411 | 14.176 | 1.00 | 59.44 | B | N |
| ATOM | 6091 | C | ASN | 317 | 89.102 | 62.140 | 11.831 | 1.00 | 38.90 | B | C |
| ATOM | 6092 | O | ASN | 317 | 89.519 | 62.549 | 10.757 | 1.00 | 39.76 | B | O |
| ATOM | 6093 | N | VAL | 318 | 88.840 | 60.858 | 12.045 | 1.00 | 40.86 | B | N |
| ATOM | 6094 | CA | VAL | 318 | 89.027 | 59.872 | 10.981 | 1.00 | 39.49 | B | C |
| ATOM | 6095 | CB | VAL | 318 | 90.348 | 59.096 | 11.156 | 1.00 | 59.32 | B | C |
| ATOM | 6096 | CG1 | VAL | 318 | 90.497 | 58.075 | 10.065 | 1.00 | 59.45 | B | C |
| ATOM | 6097 | CG2 | VAL | 318 | 91.519 | 60.052 | 11.111 | 1.00 | 59.30 | B | C |
| ATOM | 6098 | C | VAL | 318 | 87.861 | 58.894 | 10.987 | 1.00 | 34.64 | B | C |
| ATOM | 6099 | O | VAL | 318 | 87.363 | 58.523 | 12.050 | 1.00 | 35.31 | B | O |
| ATOM | 6100 | N | SER | 319 | 87.417 | 58.482 | 9.803 | 1.00 | 25.74 | B | N |
| ATOM | 6101 | CA | SER | 319 | 86.300 | 57.557 | 9.711 | 1.00 | 25.00 | B | C |
| ATOM | 6102 | CB | SER | 319 | 85.769 | 57.502 | 8.275 | 1.00 | 46.83 | B | C |
| ATOM | 6103 | OG | SER | 319 | 86.801 | 57.222 | 7.348 | 1.00 | 58.78 | B | O |
| ATOM | 6104 | C | SER | 319 | 86.672 | 56.161 | 10.195 | 1.00 | 23.60 | B | C |
| ATOM | 6105 | O | SER | 319 | 85.877 | 55.513 | 10.876 | 1.00 | 21.67 | B | O |
| ATOM | 6106 | N | ASP | 320 | 87.875 | 55.702 | 9.855 | 1.00 | 29.04 | B | N |
| ATOM | 6107 | CA | ASP | 320 | 88.342 | 54.377 | 10.272 | 1.00 | 29.02 | B | C |
| ATOM | 6108 | CB | ASP | 320 | 87.700 | 53.292 | 9.391 | 1.00 | 54.50 | B | C |
| ATOM | 6109 | CG | ASP | 320 | 88.036 | 53.455 | 7.907 | 1.00 | 52.95 | B | C |
| ATOM | 6110 | OD1 | ASP | 320 | 87.708 | 54.505 | 7.318 | 1.00 | 51.63 | B | O |
| ATOM | 6111 | OD2 | ASP | 320 | 88.628 | 52.525 | 7.324 | 1.00 | 53.50 | B | O |
| ATOM | 6112 | C | ASP | 320 | 89.878 | 54.249 | 10.227 | 1.00 | 27.39 | B | C |
| ATOM | 6113 | O | ASP | 320 | 90.574 | 55.142 | 9.734 | 1.00 | 27.17 | B | O |
| ATOM | 6114 | N | GLU | 321 | 90.403 | 53.140 | 10.745 | 1.00 | 32.71 | B | N |
| ATOM | 6115 | CA | GLU | 321 | 91.845 | 52.909 | 10.748 | 1.00 | 33.69 | B | C |
| ATOM | 6116 | CB | GLU | 321 | 92.152 | 51.430 | 11.018 | 1.00 | 76.40 | B | C |
| ATOM | 6117 | CG | GLU | 321 | 92.439 | 51.066 | 12.469 | 1.00 | 70.24 | B | C |
| ATOM | 6118 | CD | GLU | 321 | 91.229 | 51.194 | 13.373 | 1.00 | 69.99 | B | C |
| ATOM | 6119 | OE1 | GLU | 321 | 90.159 | 50.621 | 13.053 | 1.00 | 71.42 | B | O |
| ATOM | 6120 | OE2 | GLU | 321 | 91.357 | 51.862 | 14.418 | 1.00 | 74.03 | B | O |
| ATOM | 6121 | C | GLU | 321 | 92.476 | 53.300 | 9.412 | 1.00 | 37.68 | B | C |
| ATOM | 6122 | O | GLU | 321 | 93.529 | 53.943 | 9.369 | 1.00 | 34.44 | B | O |
| ATOM | 6123 | N | LEU | 322 | 91.820 | 52.905 | 8.323 | 1.00 | 34.24 | B | N |
| ATOM | 6124 | CA | LEU | 322 | 92.310 | 53.175 | 6.971 | 1.00 | 36.93 | B | C |
| ATOM | 6125 | CB | LEU | 322 | 91.345 | 52.598 | 5.937 | 1.00 | 67.00 | B | C |
| ATOM | 6126 | CG | LEU | 322 | 91.361 | 51.081 | 5.743 | 1.00 | 65.63 | B | C |
| ATOM | 6127 | CD1 | LEU | 322 | 92.716 | 50.681 | 5.198 | 1.00 | 67.37 | B | C |
| ATOM | 6128 | CD2 | LEU | 322 | 91.058 | 50.353 | 7.063 | 1.00 | 70.68 | B | C |
| ATOM | 6129 | C | LEU | 322 | 92.566 | 54.632 | 6.643 | 1.00 | 38.52 | B | C |
| ATOM | 6130 | O | LEU | 322 | 93.607 | 54.971 | 6.097 | 1.00 | 41.87 | B | O |
| ATOM | 6131 | N | ALA | 323 | 91.617 | 55.492 | 6.974 | 1.00 | 34.22 | B | N |
| ATOM | 6132 | CA | ALA | 323 | 91.759 | 56.908 | 6.687 | 1.00 | 34.65 | B | C |

Fig. 19: A-85

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 6133 | CB | ALA | 323 | 90.420 | 57.600 | 6.897 | 1.00 | 1.87 | B | C |
| ATOM | 6134 | C | ALA | 323 | 92.859 | 57.644 | 7.476 | 1.00 | 35.06 | B | C |
| ATOM | 6135 | O | ALA | 323 | 93.171 | 58.804 | 7.181 | 1.00 | 35.08 | B | O |
| ATOM | 6136 | N | LEU | 324 | 93.447 | 56.995 | 8.476 | 1.00 | 26.80 | B | N |
| ATOM | 6137 | CA | LEU | 324 | 94.492 | 57.652 | 9.256 | 1.00 | 25.28 | B | C |
| ATOM | 6138 | CB | LEU | 324 | 95.221 | 56.640 | 10.146 | 1.00 | 29.36 | B | C |
| ATOM | 6139 | CG | LEU | 324 | 94.590 | 56.344 | 11.516 | 1.00 | 28.09 | B | C |
| ATOM | 6140 | CD1 | LEU | 324 | 95.288 | 55.158 | 12.170 | 1.00 | 27.23 | B | C |
| ATOM | 6141 | CD2 | LEU | 324 | 94.676 | 57.580 | 12.406 | 1.00 | 26.02 | B | C |
| ATOM | 6142 | C | LEU | 324 | 95.495 | 58.366 | 8.354 | 1.00 | 28.81 | B | C |
| ATOM | 6143 | O | LEU | 324 | 95.822 | 59.521 | 8.588 | 1.00 | 25.35 | B | O |
| ATOM | 6144 | N | VAL | 325 | 95.966 | 57.679 | 7.317 | 1.00 | 52.77 | B | N |
| ATOM | 6145 | CA | VAL | 325 | 96.934 | 58.246 | 6.378 | 1.00 | 56.30 | B | C |
| ATOM | 6146 | CB | VAL | 325 | 97.153 | 57.321 | 5.185 | 1.00 | 36.74 | B | C |
| ATOM | 6147 | CG1 | VAL | 325 | 97.936 | 56.099 | 5.614 | 1.00 | 36.85 | B | C |
| ATOM | 6148 | CG2 | VAL | 325 | 95.810 | 56.923 | 4.599 | 1.00 | 40.13 | B | C |
| ATOM | 6149 | C | VAL | 325 | 96.524 | 59.598 | 5.818 | 1.00 | 59.12 | B | C |
| ATOM | 6150 | O | VAL | 325 | 97.324 | 60.529 | 5.761 | 1.00 | 61.18 | B | O |
| ATOM | 6151 | N | THR | 326 | 95.277 | 59.694 | 5.384 | 1.00 | 40.34 | B | N |
| ATOM | 6152 | CA | THR | 326 | 94.743 | 60.925 | 4.818 | 1.00 | 41.75 | B | C |
| ATOM | 6153 | CB | THR | 326 | 93.298 | 60.706 | 4.344 | 1.00 | 81.94 | B | C |
| ATOM | 6154 | OG1 | THR | 326 | 92.430 | 60.600 | 5.481 | 1.00 | 83.85 | B | O |
| ATOM | 6155 | CG2 | THR | 326 | 93.206 | 59.417 | 3.534 | 1.00 | 84.31 | B | C |
| ATOM | 6156 | C | THR | 326 | 94.744 | 62.070 | 5.836 | 1.00 | 41.76 | B | C |
| ATOM | 6157 | O | THR | 326 | 93.885 | 62.952 | 5.785 | 1.00 | 40.58 | B | O |
| ATOM | 6158 | N | ILE | 327 | 95.705 | 62.052 | 6.755 | 1.00 | 36.65 | B | N |
| ATOM | 6159 | CA | ILE | 327 | 95.812 | 63.075 | 7.792 | 1.00 | 36.84 | B | C |
| ATOM | 6160 | CB | ILE | 327 | 95.078 | 62.604 | 9.085 | 1.00 | 16.25 | B | C |
| ATOM | 6161 | CG2 | ILE | 327 | 95.934 | 62.757 | 10.328 | 1.00 | 17.02 | B | C |
| ATOM | 6162 | CG1 | ILE | 327 | 93.807 | 63.408 | 9.260 | 1.00 | 16.61 | B | C |
| ATOM | 6163 | CD1 | ILE | 327 | 92.943 | 62.878 | 10.372 | 1.00 | 16.28 | B | C |
| ATOM | 6164 | C | ILE | 327 | 97.272 | 63.402 | 8.093 | 1.00 | 37.35 | B | C |
| ATOM | 6165 | O | ILE | 327 | 97.590 | 64.494 | 8.559 | 1.00 | 37.60 | B | O |
| ATOM | 6166 | N | VAL | 328 | 98.158 | 62.455 | 7.804 | 1.00 | 43.89 | B | N |
| ATOM | 6167 | CA | VAL | 328 | 99.575 | 62.643 | 8.060 | 1.00 | 46.03 | B | C |
| ATOM | 6168 | CB | VAL | 328 | 100.407 | 61.469 | 7.510 | 1.00 | 54.81 | B | C |
| ATOM | 6169 | CG1 | VAL | 328 | 99.871 | 60.157 | 8.061 | 1.00 | 56.76 | B | C |
| ATOM | 6170 | CG2 | VAL | 328 | 100.381 | 61.480 | 5.997 | 1.00 | 56.08 | B | C |
| ATOM | 6171 | C | VAL | 328 | 100.121 | 63.943 | 7.481 | 1.00 | 45.95 | B | C |
| ATOM | 6172 | O | VAL | 328 | 100.998 | 64.563 | 8.075 | 1.00 | 45.23 | B | O |
| ATOM | 6173 | N | LYS | 329 | 99.611 | 64.366 | 6.331 | 1.00 | 44.51 | B | N |
| ATOM | 6174 | CA | LYS | 329 | 100.097 | 65.609 | 5.732 | 1.00 | 43.72 | B | C |
| ATOM | 6175 | CB | LYS | 329 | 99.471 | 65.824 | 4.356 | 1.00 | 45.34 | B | C |
| ATOM | 6176 | CG | LYS | 329 | 100.174 | 66.880 | 3.520 | 1.00 | 46.89 | B | C |
| ATOM | 6177 | CD | LYS | 329 | 99.423 | 67.129 | 2.220 | 1.00 | 49.21 | B | C |
| ATOM | 6178 | CE | LYS | 329 | 100.179 | 68.074 | 1.298 | 1.00 | 52.25 | B | C |
| ATOM | 6179 | NZ | LYS | 329 | 101.450 | 67.466 | 0.831 | 1.00 | 55.93 | B | N |
| ATOM | 6180 | C | LYS | 329 | 99.762 | 66.797 | 6.640 | 1.00 | 41.89 | B | C |
| ATOM | 6181 | O | LYS | 329 | 100.640 | 67.552 | 7.056 | 1.00 | 43.10 | B | O |
| ATOM | 6182 | N | ALA | 330 | 98.483 | 66.957 | 6.952 | 1.00 | 14.46 | B | N |
| ATOM | 6183 | CA | ALA | 330 | 98.053 | 68.043 | 7.814 | 1.00 | 14.49 | B | C |
| ATOM | 6184 | CB | ALA | 330 | 96.538 | 68.052 | 7.906 | 1.00 | 26.19 | B | C |
| ATOM | 6185 | C | ALA | 330 | 98.657 | 67.910 | 9.210 | 1.00 | 15.64 | B | C |
| ATOM | 6186 | O | ALA | 330 | 99.090 | 68.896 | 9.796 | 1.00 | 15.54 | B | O |
| ATOM | 6187 | N | LEU | 331 | 98.666 | 66.688 | 9.745 | 1.00 | 29.61 | B | N |
| ATOM | 6188 | CA | LEU | 331 | 99.200 | 66.447 | 11.078 | 1.00 | 27.25 | B | C |
| ATOM | 6189 | CB | LEU | 331 | 99.108 | 64.969 | 11.454 | 1.00 | 20.84 | B | C |
| ATOM | 6190 | CG | LEU | 331 | 99.086 | 64.642 | 12.958 | 1.00 | 17.26 | B | C |
| ATOM | 6191 | CD1 | LEU | 331 | 99.332 | 63.152 | 13.131 | 1.00 | 18.89 | B | C |
| ATOM | 6192 | CD2 | LEU | 331 | 100.130 | 65.436 | 13.722 | 1.00 | 12.95 | B | C |
| ATOM | 6193 | C | LEU | 331 | 100.647 | 66.860 | 11.070 | 1.00 | 27.28 | B | C |
| ATOM | 6194 | O | LEU | 331 | 101.090 | 67.613 | 11.931 | 1.00 | 26.63 | B | O |
| ATOM | 6195 | N | GLY | 332 | 101.374 | 66.358 | 10.079 | 1.00 | 36.12 | B | N |
| ATOM | 6196 | CA | GLY | 332 | 102.784 | 66.666 | 9.949 | 1.00 | 37.22 | B | C |
| ATOM | 6197 | C | GLY | 332 | 103.089 | 68.150 | 9.917 | 1.00 | 37.48 | B | C |
| ATOM | 6198 | O | GLY | 332 | 103.940 | 68.628 | 10.670 | 1.00 | 41.35 | B | O |
| ATOM | 6199 | N | GLU | 333 | 102.398 | 68.892 | 9.058 | 1.00 | 41.72 | B | N |
| ATOM | 6200 | CA | GLU | 333 | 102.653 | 70.317 | 8.967 | 1.00 | 39.78 | B | C |
| ATOM | 6201 | CB | GLU | 333 | 102.052 | 70.889 | 7.683 | 1.00 | 98.89 | B | C |
| ATOM | 6202 | CG | GLU | 333 | 100.546 | 70.988 | 7.678 | 1.00 | 97.26 | B | C |
| ATOM | 6203 | CD | GLU | 333 | 100.018 | 71.598 | 6.400 | 1.00 | 97.28 | B | C |
| ATOM | 6204 | OE1 | GLU | 333 | 98.795 | 71.849 | 6.322 | 1.00 | 99.33 | B | O |
| ATOM | 6205 | OE2 | GLU | 333 | 100.824 | 71.823 | 5.472 | 1.00 | 91.40 | B | O |

Fig. 19: A-86

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 6206 | C | GLU | 333 | 102.120 | 71.069 | 10.179 | 1.00 | 38.76 | B | C |
| ATOM | 6207 | O | GLU | 333 | 102.747 | 72.010 | 10.650 | 1.00 | 38.38 | B | O |
| ATOM | 6208 | N | ARG | 334 | 100.969 | 70.659 | 10.695 | 1.00 | 43.09 | B | N |
| ATOM | 6209 | CA | ARG | 334 | 100.398 | 71.340 | 11.847 | 1.00 | 46.47 | B | C |
| ATOM | 6210 | CB | ARG | 334 | 99.089 | 70.667 | 12.265 | 1.00 | 41.05 | B | C |
| ATOM | 6211 | CG | ARG | 334 | 98.167 | 71.568 | 13.056 | 1.00 | 40.34 | B | C |
| ATOM | 6212 | CD | ARG | 334 | 96.722 | 71.432 | 12.592 | 1.00 | 39.10 | B | C |
| ATOM | 6213 | NE | ARG | 334 | 96.544 | 71.911 | 11.222 | 1.00 | 34.65 | B | N |
| ATOM | 6214 | CZ | ARG | 334 | 95.446 | 71.721 | 10.488 | 1.00 | 38.74 | B | C |
| ATOM | 6215 | NH1 | ARG | 334 | 94.407 | 71.052 | 10.987 | 1.00 | 35.48 | B | N |
| ATOM | 6216 | NH2 | ARG | 334 | 95.388 | 72.197 | 9.246 | 1.00 | 44.88 | B | N |
| ATOM | 6217 | C | ARG | 334 | 101.419 | 71.321 | 12.980 | 1.00 | 47.77 | B | C |
| ATOM | 6218 | O | ARG | 334 | 101.633 | 72.329 | 13.643 | 1.00 | 44.69 | B | O |
| ATOM | 6219 | N | ILE | 335 | 102.060 | 70.177 | 13.192 | 1.00 | 95.68 | B | N |
| ATOM | 6220 | CA | ILE | 335 | 103.084 | 70.066 | 14.227 | 1.00 | 95.61 | B | C |
| ATOM | 6221 | CB | ILE | 335 | 103.349 | 68.565 | 14.599 | 1.00 | 69.44 | B | C |
| ATOM | 6222 | CG2 | ILE | 335 | 103.371 | 67.701 | 13.359 | 1.00 | 72.22 | B | C |
| ATOM | 6223 | CG1 | ILE | 335 | 104.671 | 68.420 | 15.350 | 1.00 | 70.66 | B | C |
| ATOM | 6224 | CD1 | ILE | 335 | 105.043 | 66.983 | 15.628 | 1.00 | 73.45 | B | C |
| ATOM | 6225 | C | ILE | 335 | 104.346 | 70.716 | 13.653 | 1.00 | 93.90 | B | C |
| ATOM | 6226 | O | ILE | 335 | 105.317 | 70.979 | 14.364 | 1.00 | 96.50 | B | O |
| ATOM | 6227 | N | PHE | 336 | 104.273 | 71.011 | 12.356 | 1.00 | 144.26 | B | N |
| ATOM | 6228 | CA | PHE | 336 | 105.347 | 71.604 | 11.560 | 1.00 | 143.89 | B | C |
| ATOM | 6229 | CB | PHE | 336 | 105.336 | 73.156 | 11.625 | 1.00 | 83.50 | B | C |
| ATOM | 6230 | CG | PHE | 336 | 105.600 | 73.748 | 12.992 | 1.00 | 79.82 | B | C |
| ATOM | 6231 | CD1 | PHE | 336 | 106.696 | 73.355 | 13.760 | 1.00 | 79.24 | B | C |
| ATOM | 6232 | CD2 | PHE | 336 | 104.783 | 74.762 | 13.479 | 1.00 | 77.77 | B | C |
| ATOM | 6233 | CE1 | PHE | 336 | 106.973 | 73.966 | 14.988 | 1.00 | 69.57 | B | C |
| ATOM | 6234 | CE2 | PHE | 336 | 105.053 | 75.377 | 14.702 | 1.00 | 72.13 | B | C |
| ATOM | 6235 | CZ | PHE | 336 | 106.152 | 74.977 | 15.457 | 1.00 | 72.59 | B | C |
| ATOM | 6236 | C | PHE | 336 | 106.737 | 71.068 | 11.853 | 1.00 | 143.92 | B | C |
| ATOM | 6237 | O | PHE | 336 | 106.889 | 70.255 | 12.788 | 1.00 | 123.54 | B | O |
| ATOM | 6238 | OXT | PHE | 336 | 107.658 | 71.461 | 11.111 | 1.00 | 66.99 | B | O |
| ATOM | 6239 | CB | GLU | 1 | 68.990 | 38.972 | 10.337 | 1.00 | 143.47 | X | C |
| ATOM | 6240 | CG | GLU | 1 | 68.785 | 37.653 | 11.053 | 1.00 | 143.47 | X | C |
| ATOM | 6241 | CD | GLU | 1 | 68.300 | 36.572 | 10.118 | 1.00 | 143.47 | X | C |
| ATOM | 6242 | OE1 | GLU | 1 | 69.012 | 36.278 | 9.134 | 1.00 | 143.47 | X | O |
| ATOM | 6243 | OE2 | GLU | 1 | 67.209 | 36.019 | 10.363 | 1.00 | 143.47 | X | O |
| ATOM | 6244 | C | GLU | 1 | 71.024 | 39.462 | 11.710 | 1.00 | 74.19 | X | C |
| ATOM | 6245 | O | GLU | 1 | 71.492 | 38.415 | 11.265 | 1.00 | 74.19 | X | O |
| ATOM | 6246 | N | GLU | 1 | 69.921 | 41.257 | 10.328 | 1.00 | 74.19 | X | N |
| ATOM | 6247 | CA | GLU | 1 | 69.711 | 40.037 | 11.162 | 1.00 | 74.19 | X | C |
| ATOM | 6248 | N | VAL | 2 | 71.613 | 40.151 | 12.681 | 1.00 | 55.61 | X | N |
| ATOM | 6249 | CA | VAL | 2 | 72.858 | 39.694 | 13.284 | 1.00 | 55.61 | X | C |
| ATOM | 6250 | CB | VAL | 2 | 73.533 | 40.812 | 14.089 | 1.00 | 66.95 | X | C |
| ATOM | 6251 | CG1 | VAL | 2 | 74.850 | 40.323 | 14.647 | 1.00 | 66.95 | X | C |
| ATOM | 6252 | CG2 | VAL | 2 | 73.752 | 42.021 | 13.210 | 1.00 | 66.95 | X | C |
| ATOM | 6253 | C | VAL | 2 | 72.566 | 38.543 | 14.232 | 1.00 | 55.61 | X | C |
| ATOM | 6254 | O | VAL | 2 | 71.728 | 38.673 | 15.127 | 1.00 | 55.61 | X | O |
| ATOM | 6255 | N | GLN | 3 | 73.258 | 37.421 | 14.045 | 1.00 | 39.72 | X | N |
| ATOM | 6256 | CA | GLN | 3 | 73.044 | 36.261 | 14.908 | 1.00 | 39.72 | X | C |
| ATOM | 6257 | CB | GLN | 3 | 71.807 | 35.502 | 14.455 | 1.00 | 102.66 | X | C |
| ATOM | 6258 | CG | GLN | 3 | 71.852 | 35.144 | 13.002 | 1.00 | 102.66 | X | C |
| ATOM | 6259 | CD | GLN | 3 | 70.688 | 34.291 | 12.604 | 1.00 | 102.66 | X | C |
| ATOM | 6260 | OE1 | GLN | 3 | 69.537 | 34.635 | 12.873 | 1.00 | 102.66 | X | O |
| ATOM | 6261 | NE2 | GLN | 3 | 70.972 | 33.168 | 11.955 | 1.00 | 102.66 | X | N |
| ATOM | 6262 | C | GLN | 3 | 74.213 | 35.288 | 15.002 | 1.00 | 39.72 | X | C |
| ATOM | 6263 | O | GLN | 3 | 75.064 | 35.207 | 14.108 | 1.00 | 39.72 | X | O |
| ATOM | 6264 | N | LEU | 4 | 74.231 | 34.553 | 16.109 | 1.00 | 34.59 | X | N |
| ATOM | 6265 | CA | LEU | 4 | 75.260 | 33.555 | 16.389 | 1.00 | 34.59 | X | C |
| ATOM | 6266 | CB | LEU | 4 | 76.043 | 33.931 | 17.653 | 1.00 | 34.08 | X | C |
| ATOM | 6267 | CG | LEU | 4 | 77.107 | 35.040 | 17.665 | 1.00 | 34.08 | X | C |
| ATOM | 6268 | CD1 | LEU | 4 | 77.119 | 35.820 | 16.353 | 1.00 | 34.08 | X | C |
| ATOM | 6269 | CD2 | LEU | 4 | 76.844 | 35.950 | 18.863 | 1.00 | 34.08 | X | C |
| ATOM | 6270 | C | LEU | 4 | 74.581 | 32.212 | 16.615 | 1.00 | 34.59 | X | C |
| ATOM | 6271 | O | LEU | 4 | 73.737 | 32.080 | 17.503 | 1.00 | 34.59 | X | O |
| ATOM | 6272 | N | VAL | 5 | 74.933 | 31.218 | 15.806 | 1.00 | 36.99 | X | N |
| ATOM | 6273 | CA | VAL | 5 | 74.350 | 29.889 | 15.961 | 1.00 | 36.99 | X | C |
| ATOM | 6274 | CB | VAL | 5 | 73.536 | 29.456 | 14.698 | 1.00 | 37.13 | X | C |
| ATOM | 6275 | CG1 | VAL | 5 | 74.285 | 29.815 | 13.430 | 1.00 | 37.13 | X | C |
| ATOM | 6276 | CG2 | VAL | 5 | 73.264 | 27.963 | 14.744 | 1.00 | 37.13 | X | C |
| ATOM | 6277 | C | VAL | 5 | 75.429 | 28.861 | 16.277 | 1.00 | 36.99 | X | C |
| ATOM | 6278 | O | VAL | 5 | 76.163 | 28.404 | 15.398 | 1.00 | 36.99 | X | O |

Fig. 19: A-87

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 6279 | N | GLU | 6 | 75.519 | 28.517 | 17.555 | 1.00 | 44.32 | X | N |
| ATOM | 6280 | CA | GLU | 6 | 76.499 | 27.550 | 18.020 | 1.00 | 44.32 | X | C |
| ATOM | 6281 | CB | GLU | 6 | 76.924 | 27.884 | 19.457 | 1.00 | 53.96 | X | C |
| ATOM | 6282 | CG | GLU | 6 | 75.844 | 28.531 | 20.292 | 1.00 | 53.96 | X | C |
| ATOM | 6283 | CD | GLU | 6 | 76.340 | 28.943 | 21.659 | 1.00 | 53.96 | X | C |
| ATOM | 6284 | OE1 | GLU | 6 | 75.590 | 29.646 | 22.368 | 1.00 | 53.96 | X | O |
| ATOM | 6285 | OE2 | GLU | 6 | 77.472 | 28.561 | 22.028 | 1.00 | 53.96 | X | O |
| ATOM | 6286 | C | GLU | 6 | 76.029 | 26.095 | 17.930 | 1.00 | 44.32 | X | C |
| ATOM | 6287 | O | GLU | 6 | 74.856 | 25.813 | 17.668 | 1.00 | 44.32 | X | O |
| ATOM | 6288 | N | SER | 7 | 76.980 | 25.185 | 18.135 | 1.00 | 42.31 | X | N |
| ATOM | 6289 | CA | SER | 7 | 76.758 | 23.745 | 18.091 | 1.00 | 42.31 | X | C |
| ATOM | 6290 | CB | SER | 7 | 76.762 | 23.261 | 16.642 | 1.00 | 44.31 | X | C |
| ATOM | 6291 | OG | SER | 7 | 77.832 | 23.845 | 15.922 | 1.00 | 44.31 | X | O |
| ATOM | 6292 | C | SER | 7 | 77.919 | 23.123 | 18.848 | 1.00 | 42.31 | X | C |
| ATOM | 6293 | O | SER | 7 | 78.889 | 23.813 | 19.138 | 1.00 | 42.31 | X | O |
| ATOM | 6294 | N | GLY | 8 | 77.822 | 21.838 | 19.178 | 1.00 | 39.85 | X | N |
| ATOM | 6295 | CA | GLY | 8 | 78.908 | 21.177 | 19.893 | 1.00 | 39.85 | X | C |
| ATOM | 6296 | C | GLY | 8 | 78.569 | 20.747 | 21.313 | 1.00 | 39.85 | X | C |
| ATOM | 6297 | O | GLY | 8 | 79.330 | 20.016 | 21.962 | 1.00 | 39.85 | X | O |
| ATOM | 6298 | N | GLY | 9 | 77.417 | 21.199 | 21.795 | 1.00 | 54.13 | X | N |
| ATOM | 6299 | CA | GLY | 9 | 76.998 | 20.852 | 23.138 | 1.00 | 54.13 | X | C |
| ATOM | 6300 | C | GLY | 9 | 76.467 | 19.439 | 23.283 | 1.00 | 54.13 | X | C |
| ATOM | 6301 | O | GLY | 9 | 75.390 | 19.102 | 22.783 | 1.00 | 54.13 | X | O |
| ATOM | 6302 | N | GLY | 10 | 77.235 | 18.606 | 23.972 | 1.00 | 51.55 | X | N |
| ATOM | 6303 | CA | GLY | 10 | 76.825 | 17.236 | 24.195 | 1.00 | 51.55 | X | C |
| ATOM | 6304 | C | GLY | 10 | 77.359 | 16.807 | 25.544 | 1.00 | 51.55 | X | C |
| ATOM | 6305 | O | GLY | 10 | 77.723 | 17.651 | 26.370 | 1.00 | 51.55 | X | O |
| ATOM | 6306 | N | LEU | 11 | 77.409 | 15.500 | 25.776 | 1.00 | 54.73 | X | N |
| ATOM | 6307 | CA | LEU | 11 | 77.930 | 14.981 | 27.032 | 1.00 | 54.73 | X | C |
| ATOM | 6308 | CB | LEU | 11 | 76.994 | 13.903 | 27.583 | 1.00 | 40.69 | X | C |
| ATOM | 6309 | CG | LEU | 11 | 77.583 | 13.086 | 28.735 | 1.00 | 40.69 | X | C |
| ATOM | 6310 | CD1 | LEU | 11 | 78.170 | 14.011 | 29.795 | 1.00 | 40.69 | X | C |
| ATOM | 6311 | CD2 | LEU | 11 | 76.508 | 12.198 | 29.317 | 1.00 | 40.69 | X | C |
| ATOM | 6312 | C | LEU | 11 | 79.341 | 14.412 | 26.852 | 1.00 | 54.73 | X | C |
| ATOM | 6313 | O | LEU | 11 | 79.664 | 13.853 | 25.806 | 1.00 | 54.73 | X | O |
| ATOM | 6314 | N | VAL | 12 | 80.177 | 14.576 | 27.872 | 1.00 | 43.40 | X | N |
| ATOM | 6315 | CA | VAL | 12 | 81.552 | 14.079 | 27.848 | 1.00 | 43.40 | X | C |
| ATOM | 6316 | CB | VAL | 12 | 82.538 | 15.118 | 27.273 | 1.00 | 57.73 | X | C |
| ATOM | 6317 | CG1 | VAL | 12 | 82.222 | 15.388 | 25.812 | 1.00 | 57.73 | X | C |
| ATOM | 6318 | CG2 | VAL | 12 | 82.473 | 16.404 | 28.086 | 1.00 | 57.73 | X | C |
| ATOM | 6319 | C | VAL | 12 | 81.991 | 13.753 | 29.269 | 1.00 | 43.40 | X | C |
| ATOM | 6320 | O | VAL | 12 | 81.490 | 14.344 | 30.230 | 1.00 | 43.40 | X | O |
| ATOM | 6321 | N | GLN | 13 | 82.931 | 12.821 | 29.403 | 1.00 | 46.11 | X | N |
| ATOM | 6322 | CA | GLN | 13 | 83.404 | 12.420 | 30.720 | 1.00 | 46.11 | X | C |
| ATOM | 6323 | CB | GLN | 13 | 83.873 | 10.965 | 30.676 | 1.00 | 148.60 | X | C |
| ATOM | 6324 | CG | GLN | 13 | 82.843 | 10.015 | 30.094 | 1.00 | 148.60 | X | C |
| ATOM | 6325 | CD | GLN | 13 | 83.232 | 8.560 | 30.263 | 1.00 | 148.60 | X | C |
| ATOM | 6326 | OE1 | GLN | 13 | 84.322 | 8.145 | 29.868 | 1.00 | 148.60 | X | O |
| ATOM | 6327 | NE2 | GLN | 13 | 82.337 | 7.774 | 30.852 | 1.00 | 148.60 | X | N |
| ATOM | 6328 | C | GLN | 13 | 84.532 | 13.311 | 31.234 | 1.00 | 46.11 | X | C |
| ATOM | 6329 | O | GLN | 13 | 85.186 | 14.002 | 30.454 | 1.00 | 46.11 | X | O |
| ATOM | 6330 | N | PRO | 14 | 84.763 | 13.319 | 32.563 | 1.00 | 39.23 | X | N |
| ATOM | 6331 | CD | PRO | 14 | 83.989 | 12.657 | 33.630 | 1.00 | 55.62 | X | C |
| ATOM | 6332 | CA | PRO | 14 | 85.831 | 14.141 | 33.141 | 1.00 | 39.23 | X | C |
| ATOM | 6333 | CB | PRO | 14 | 85.902 | 13.648 | 34.581 | 1.00 | 55.62 | X | C |
| ATOM | 6334 | CG | PRO | 14 | 84.474 | 13.374 | 34.887 | 1.00 | 55.62 | X | C |
| ATOM | 6335 | C | PRO | 14 | 87.122 | 13.905 | 32.392 | 1.00 | 39.23 | X | C |
| ATOM | 6336 | O | PRO | 14 | 87.357 | 12.810 | 31.885 | 1.00 | 39.23 | X | O |
| ATOM | 6337 | N | GLY | 15 | 87.954 | 14.935 | 32.320 | 1.00 | 28.04 | X | N |
| ATOM | 6338 | CA | GLY | 15 | 89.220 | 14.816 | 31.616 | 1.00 | 28.04 | X | C |
| ATOM | 6339 | C | GLY | 15 | 89.037 | 14.807 | 30.109 | 1.00 | 28.04 | X | C |
| ATOM | 6340 | O | GLY | 15 | 89.990 | 14.979 | 29.352 | 1.00 | 28.04 | X | O |
| ATOM | 6341 | N | GLY | 16 | 87.801 | 14.613 | 29.672 | 1.00 | 22.75 | X | N |
| ATOM | 6342 | CA | GLY | 16 | 87.529 | 14.583 | 28.250 | 1.00 | 22.75 | X | C |
| ATOM | 6343 | C | GLY | 16 | 87.705 | 15.912 | 27.539 | 1.00 | 22.75 | X | C |
| ATOM | 6344 | O | GLY | 16 | 87.887 | 16.969 | 28.155 | 1.00 | 22.75 | X | O |
| ATOM | 6345 | N | SER | 17 | 87.633 | 15.845 | 26.217 | 1.00 | 36.95 | X | N |
| ATOM | 6346 | CA | SER | 17 | 87.789 | 17.014 | 25.371 | 1.00 | 36.95 | X | C |
| ATOM | 6347 | CB | SER | 17 | 88.962 | 16.795 | 24.417 | 1.00 | 47.78 | X | C |
| ATOM | 6348 | OG | SER | 17 | 89.203 | 17.952 | 23.645 | 1.00 | 47.78 | X | O |
| ATOM | 6349 | C | SER | 17 | 86.509 | 17.311 | 24.581 | 1.00 | 36.95 | X | C |
| ATOM | 6350 | O | SER | 17 | 85.817 | 16.402 | 24.106 | 1.00 | 36.95 | X | O |
| ATOM | 6351 | N | LEU | 18 | 86.199 | 18.593 | 24.429 | 1.00 | 50.75 | X | N |

Fig. 19: A-88

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 6352 | CA | LEU | 18 | 84.995 | 18.978 | 23.719 | 1.00 | 50.75 | X | C |
| ATOM | 6353 | CB | LEU | 18 | 83.833 | 18.944 | 24.701 | 1.00 | 37.38 | X | C |
| ATOM | 6354 | CG | LEU | 18 | 82.463 | 19.285 | 24.146 | 1.00 | 37.38 | X | C |
| ATOM | 6355 | CD1 | LEU | 18 | 82.177 | 18.476 | 22.874 | 1.00 | 37.38 | X | C |
| ATOM | 6356 | CD2 | LEU | 18 | 81.442 | 19.012 | 25.239 | 1.00 | 37.38 | X | C |
| ATOM | 6357 | C | LEU | 18 | 85.107 | 20.355 | 23.069 | 1.00 | 50.75 | X | C |
| ATOM | 6358 | O | LEU | 18 | 85.530 | 21.313 | 23.714 | 1.00 | 50.75 | X | O |
| ATOM | 6359 | N | ARG | 19 | 84.737 | 20.454 | 21.792 | 1.00 | 27.07 | X | N |
| ATOM | 6360 | CA | ARG | 19 | 84.805 | 21.739 | 21.097 | 1.00 | 27.07 | X | C |
| ATOM | 6361 | CB | ARG | 19 | 85.774 | 21.708 | 19.924 | 1.00 | 43.18 | X | C |
| ATOM | 6362 | CG | ARG | 19 | 85.825 | 23.068 | 19.238 | 1.00 | 43.18 | X | C |
| ATOM | 6363 | CD | ARG | 19 | 86.689 | 23.075 | 18.015 | 1.00 | 43.18 | X | C |
| ATOM | 6364 | NE | ARG | 19 | 86.060 | 22.389 | 16.896 | 1.00 | 43.18 | X | N |
| ATOM | 6365 | CZ | ARG | 19 | 86.564 | 22.371 | 15.666 | 1.00 | 43.18 | X | C |
| ATOM | 6366 | NH1 | ARG | 19 | 87.708 | 23.006 | 15.407 | 1.00 | 43.18 | X | N |
| ATOM | 6367 | NH2 | ARG | 19 | 85.924 | 21.725 | 14.696 | 1.00 | 43.18 | X | N |
| ATOM | 6368 | C | ARG | 19 | 83.501 | 22.302 | 20.558 | 1.00 | 27.07 | X | C |
| ATOM | 6369 | O | ARG | 19 | 82.895 | 21.745 | 19.625 | 1.00 | 27.07 | X | O |
| ATOM | 6370 | N | LEU | 20 | 83.109 | 23.438 | 21.135 | 1.00 | 30.57 | X | N |
| ATOM | 6371 | CA | LEU | 20 | 81.908 | 24.150 | 20.731 | 1.00 | 30.57 | X | C |
| ATOM | 6372 | CB | LEU | 20 | 81.354 | 24.965 | 21.896 | 1.00 | 36.53 | X | C |
| ATOM | 6373 | CG | LEU | 20 | 80.981 | 24.196 | 23.159 | 1.00 | 36.53 | X | C |
| ATOM | 6374 | CD1 | LEU | 20 | 80.415 | 25.142 | 24.218 | 1.00 | 36.53 | X | C |
| ATOM | 6375 | CD2 | LEU | 20 | 79.964 | 23.135 | 22.802 | 1.00 | 36.53 | X | C |
| ATOM | 6376 | C | LEU | 20 | 82.304 | 25.098 | 19.618 | 1.00 | 30.57 | X | C |
| ATOM | 6377 | O | LEU | 20 | 83.313 | 25.784 | 19.723 | 1.00 | 30.57 | X | O |
| ATOM | 6378 | N | SER | 21 | 81.527 | 25.122 | 18.544 | 1.00 | 31.77 | X | N |
| ATOM | 6379 | CA | SER | 21 | 81.789 | 26.024 | 17.426 | 1.00 | 31.77 | X | C |
| ATOM | 6380 | CB | SER | 21 | 81.876 | 25.252 | 16.117 | 1.00 | 32.65 | X | C |
| ATOM | 6381 | OG | SER | 21 | 80.580 | 24.896 | 15.682 | 1.00 | 32.65 | X | O |
| ATOM | 6382 | C | SER | 21 | 80.593 | 26.971 | 17.383 | 1.00 | 31.77 | X | C |
| ATOM | 6383 | O | SER | 21 | 79.591 | 26.738 | 18.057 | 1.00 | 31.77 | X | O |
| ATOM | 6384 | N | CYS | 22 | 80.673 | 28.024 | 16.585 | 1.00 | 49.03 | X | N |
| ATOM | 6385 | CA | CYS | 22 | 79.580 | 28.981 | 16.526 | 1.00 | 49.03 | X | C |
| ATOM | 6386 | C | CYS | 22 | 79.725 | 29.812 | 15.272 | 1.00 | 49.03 | X | C |
| ATOM | 6387 | O | CYS | 22 | 80.743 | 30.484 | 15.096 | 1.00 | 49.03 | X | O |
| ATOM | 6388 | CB | CYS | 22 | 79.643 | 29.849 | 17.788 | 1.00 | 49.62 | X | C |
| ATOM | 6389 | SG | CYS | 22 | 78.993 | 31.555 | 17.774 | 1.00 | 49.62 | X | S |
| ATOM | 6390 | N | ALA | 23 | 78.724 | 29.744 | 14.389 | 1.00 | 43.82 | X | N |
| ATOM | 6391 | CA | ALA | 23 | 78.742 | 30.509 | 13.136 | 1.00 | 43.82 | X | C |
| ATOM | 6392 | CB | ALA | 23 | 78.022 | 29.768 | 12.021 | 1.00 | 1.87 | X | C |
| ATOM | 6393 | C | ALA | 23 | 78.093 | 31.854 | 13.329 | 1.00 | 43.82 | X | C |
| ATOM | 6394 | O | ALA | 23 | 77.118 | 31.999 | 14.070 | 1.00 | 43.82 | X | O |
| ATOM | 6395 | N | ALA | 24 | 78.644 | 32.843 | 12.645 | 1.00 | 28.70 | X | N |
| ATOM | 6396 | CA | ALA | 24 | 78.129 | 34.190 | 12.735 | 1.00 | 28.70 | X | C |
| ATOM | 6397 | CB | ALA | 24 | 79.199 | 35.129 | 13.323 | 1.00 | 18.49 | X | C |
| ATOM | 6398 | C | ALA | 24 | 77.725 | 34.659 | 11.356 | 1.00 | 28.70 | X | C |
| ATOM | 6399 | O | ALA | 24 | 78.213 | 34.160 | 10.345 | 1.00 | 28.70 | X | O |
| ATOM | 6400 | N | SER | 25 | 76.816 | 35.620 | 11.338 | 1.00 | 39.45 | X | N |
| ATOM | 6401 | CA | SER | 25 | 76.338 | 36.218 | 10.108 | 1.00 | 39.45 | X | C |
| ATOM | 6402 | CB | SER | 25 | 75.279 | 35.322 | 9.443 | 1.00 | 48.28 | X | C |
| ATOM | 6403 | OG | SER | 25 | 74.163 | 35.090 | 10.287 | 1.00 | 48.28 | X | O |
| ATOM | 6404 | C | SER | 25 | 75.751 | 37.575 | 10.486 | 1.00 | 39.45 | X | C |
| ATOM | 6405 | O | SER | 25 | 75.425 | 37.819 | 11.656 | 1.00 | 39.45 | X | O |
| ATOM | 6406 | N | GLY | 26 | 75.651 | 38.464 | 9.506 | 1.00 | 15.13 | X | N |
| ATOM | 6407 | CA | GLY | 26 | 75.093 | 39.773 | 9.767 | 1.00 | 15.13 | X | C |
| ATOM | 6408 | C | GLY | 26 | 76.061 | 40.808 | 10.313 | 1.00 | 15.13 | X | C |
| ATOM | 6409 | O | GLY | 26 | 75.650 | 41.692 | 11.070 | 1.00 | 15.13 | X | O |
| ATOM | 6410 | N | PHE | 27 | 77.336 | 40.697 | 9.941 | 1.00 | 51.25 | X | N |
| ATOM | 6411 | CA | PHE | 27 | 78.375 | 41.638 | 10.358 | 1.00 | 51.25 | X | C |
| ATOM | 6412 | CB | PHE | 27 | 78.322 | 41.921 | 11.860 | 1.00 | 33.43 | X | C |
| ATOM | 6413 | CG | PHE | 27 | 78.647 | 40.736 | 12.720 | 1.00 | 33.43 | X | C |
| ATOM | 6414 | CD1 | PHE | 27 | 77.696 | 39.749 | 12.958 | 1.00 | 33.43 | X | C |
| ATOM | 6415 | CD2 | PHE | 27 | 79.891 | 40.629 | 13.337 | 1.00 | 33.43 | X | C |
| ATOM | 6416 | CE1 | PHE | 27 | 77.978 | 38.673 | 13.810 | 1.00 | 33.43 | X | C |
| ATOM | 6417 | CE2 | PHE | 27 | 80.186 | 39.558 | 14.190 | 1.00 | 33.43 | X | C |
| ATOM | 6418 | CZ | PHE | 27 | 79.227 | 38.581 | 14.428 | 1.00 | 33.43 | X | C |
| ATOM | 6419 | C | PHE | 27 | 79.748 | 41.100 | 10.012 | 1.00 | 51.25 | X | C |
| ATOM | 6420 | O | PHE | 27 | 79.966 | 39.894 | 10.027 | 1.00 | 51.25 | X | O |
| ATOM | 6421 | N | THR | 28 | 80.671 | 42.006 | 9.707 | 1.00 | 31.93 | X | N |
| ATOM | 6422 | CA | THR | 28 | 82.031 | 41.637 | 9.348 | 1.00 | 31.93 | X | C |
| ATOM | 6423 | CB | THR | 28 | 82.821 | 42.872 | 8.910 | 1.00 | 48.89 | X | C |
| ATOM | 6424 | OG1 | THR | 28 | 82.126 | 43.520 | 7.836 | 1.00 | 48.89 | X | O |

# Fig. 19: A-89

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 6425 | CG2 | THR | 28 | 84.212 | 42.474 | 8.454 | 1.00 | 48.89 | X | C |
| ATOM | 6426 | C | THR | 28 | 82.744 | 40.981 | 10.519 | 1.00 | 31.93 | X | C |
| ATOM | 6427 | O | THR | 28 | 83.431 | 41.640 | 11.286 | 1.00 | 31.93 | X | O |
| ATOM | 6428 | N | PHE | 29 | 82.576 | 39.671 | 10.636 | 1.00 | 37.68 | X | N |
| ATOM | 6429 | CA | PHE | 29 | 83.166 | 38.876 | 11.712 | 1.00 | 37.68 | X | C |
| ATOM | 6430 | CB | PHE | 29 | 83.068 | 37.386 | 11.352 | 1.00 | 38.41 | X | C |
| ATOM | 6431 | CG | PHE | 29 | 83.484 | 36.454 | 12.462 | 1.00 | 38.41 | X | C |
| ATOM | 6432 | CD1 | PHE | 29 | 82.795 | 36.440 | 13.676 | 1.00 | 38.41 | X | C |
| ATOM | 6433 | CD2 | PHE | 29 | 84.570 | 35.587 | 12.296 | 1.00 | 38.41 | X | C |
| ATOM | 6434 | CE1 | PHE | 29 | 83.183 | 35.577 | 14.709 | 1.00 | 38.41 | X | C |
| ATOM | 6435 | CE2 | PHE | 29 | 84.967 | 34.718 | 13.324 | 1.00 | 38.41 | X | C |
| ATOM | 6436 | CZ | PHE | 29 | 84.272 | 34.715 | 14.530 | 1.00 | 38.41 | X | C |
| ATOM | 6437 | C | PHE | 29 | 84.616 | 39.225 | 12.021 | 1.00 | 37.68 | X | C |
| ATOM | 6438 | O | PHE | 29 | 84.958 | 39.552 | 13.160 | 1.00 | 37.68 | X | O |
| ATOM | 6439 | N | SER | 30 | 85.462 | 39.160 | 10.998 | 1.00 | 22.05 | X | N |
| ATOM | 6440 | CA | SER | 30 | 86.890 | 39.421 | 11.157 | 1.00 | 22.05 | X | C |
| ATOM | 6441 | CB | SER | 30 | 87.553 | 39.545 | 9.783 | 1.00 | 37.79 | X | C |
| ATOM | 6442 | OG | SER | 30 | 86.886 | 40.481 | 8.959 | 1.00 | 37.79 | X | O |
| ATOM | 6443 | C | SER | 30 | 87.270 | 40.622 | 12.014 | 1.00 | 22.05 | X | C |
| ATOM | 6444 | O | SER | 30 | 88.326 | 40.634 | 12.639 | 1.00 | 22.05 | X | O |
| ATOM | 6445 | N | ARG | 31 | 86.395 | 41.615 | 12.063 | 1.00 | 29.69 | X | N |
| ATOM | 6446 | CA | ARG | 31 | 86.651 | 42.846 | 12.801 | 1.00 | 29.69 | X | C |
| ATOM | 6447 | CB | ARG | 31 | 85.819 | 43.956 | 12.162 | 1.00 | 51.15 | X | C |
| ATOM | 6448 | CG | ARG | 31 | 86.068 | 45.323 | 12.719 | 1.00 | 51.15 | X | C |
| ATOM | 6449 | CD | ARG | 31 | 84.999 | 46.281 | 12.231 | 1.00 | 51.15 | X | C |
| ATOM | 6450 | NE | ARG | 31 | 84.964 | 46.383 | 10.772 | 1.00 | 51.15 | X | N |
| ATOM | 6451 | CZ | ARG | 31 | 85.899 | 46.974 | 10.038 | 1.00 | 51.15 | X | C |
| ATOM | 6452 | NH1 | ARG | 31 | 86.959 | 47.523 | 10.621 | 1.00 | 51.15 | X | N |
| ATOM | 6453 | NH2 | ARG | 31 | 85.764 | 47.027 | 8.722 | 1.00 | 51.15 | X | N |
| ATOM | 6454 | C | ARG | 31 | 86.425 | 42.833 | 14.329 | 1.00 | 29.69 | X | C |
| ATOM | 6455 | O | ARG | 31 | 87.226 | 43.399 | 15.080 | 1.00 | 29.69 | X | O |
| ATOM | 6456 | N | TYR | 32 | 85.352 | 42.185 | 14.785 | 1.00 | 39.46 | X | N |
| ATOM | 6457 | CA | TYR | 32 | 85.009 | 42.144 | 16.217 | 1.00 | 39.46 | X | C |
| ATOM | 6458 | CB | TYR | 32 | 83.506 | 41.880 | 16.409 | 1.00 | 51.56 | X | C |
| ATOM | 6459 | CG | TYR | 32 | 82.601 | 42.689 | 15.516 | 1.00 | 51.56 | X | C |
| ATOM | 6460 | CD1 | TYR | 32 | 82.540 | 42.437 | 14.148 | 1.00 | 51.56 | X | C |
| ATOM | 6461 | CE1 | TYR | 32 | 81.721 | 43.181 | 13.316 | 1.00 | 51.56 | X | C |
| ATOM | 6462 | CD2 | TYR | 32 | 81.811 | 43.714 | 16.034 | 1.00 | 51.56 | X | C |
| ATOM | 6463 | CE2 | TYR | 32 | 80.985 | 44.467 | 15.209 | 1.00 | 51.56 | X | C |
| ATOM | 6464 | CZ | TYR | 32 | 80.946 | 44.193 | 13.851 | 1.00 | 51.56 | X | C |
| ATOM | 6465 | OH | TYR | 32 | 80.135 | 44.929 | 13.015 | 1.00 | 51.56 | X | O |
| ATOM | 6466 | C | TYR | 32 | 85.761 | 41.108 | 17.037 | 1.00 | 39.46 | X | C |
| ATOM | 6467 | O | TYR | 32 | 86.159 | 40.072 | 16.515 | 1.00 | 39.46 | X | O |
| ATOM | 6468 | N | THR | 33 | 85.943 | 41.386 | 18.328 | 1.00 | 29.44 | X | N |
| ATOM | 6469 | CA | THR | 33 | 86.611 | 40.421 | 19.191 | 1.00 | 29.44 | X | C |
| ATOM | 6470 | CB | THR | 33 | 87.510 | 41.080 | 20.315 | 1.00 | 20.65 | X | C |
| ATOM | 6471 | OG1 | THR | 33 | 86.749 | 41.242 | 21.514 | 1.00 | 20.65 | X | O |
| ATOM | 6472 | CG2 | THR | 33 | 88.072 | 42.437 | 19.866 | 1.00 | 20.65 | X | C |
| ATOM | 6473 | C | THR | 33 | 85.483 | 39.614 | 19.835 | 1.00 | 29.44 | X | C |
| ATOM | 6474 | O | THR | 33 | 84.632 | 40.167 | 20.536 | 1.00 | 29.44 | X | O |
| ATOM | 6475 | N | MET | 34 | 85.484 | 38.307 | 19.568 | 1.00 | 30.35 | X | N |
| ATOM | 6476 | CA | MET | 34 | 84.474 | 37.391 | 20.084 | 1.00 | 30.35 | X | C |
| ATOM | 6477 | CB | MET | 34 | 84.235 | 36.284 | 19.067 | 1.00 | 43.39 | X | C |
| ATOM | 6478 | CG | MET | 34 | 84.070 | 36.798 | 17.652 | 1.00 | 43.39 | X | C |
| ATOM | 6479 | SD | MET | 34 | 82.775 | 38.029 | 17.525 | 1.00 | 43.39 | X | S |
| ATOM | 6480 | CE | MET | 34 | 81.376 | 37.024 | 17.198 | 1.00 | 43.39 | X | C |
| ATOM | 6481 | C | MET | 34 | 84.867 | 36.785 | 21.430 | 1.00 | 30.35 | X | C |
| ATOM | 6482 | O | MET | 34 | 86.049 | 36.761 | 21.790 | 1.00 | 30.35 | X | O |
| ATOM | 6483 | N | SER | 35 | 83.866 | 36.293 | 22.164 | 1.00 | 35.95 | X | N |
| ATOM | 6484 | CA | SER | 35 | 84.073 | 35.701 | 23.487 | 1.00 | 35.95 | X | C |
| ATOM | 6485 | CB | SER | 35 | 83.875 | 36.765 | 24.580 | 1.00 | 34.42 | X | C |
| ATOM | 6486 | OG | SER | 35 | 84.740 | 37.878 | 24.420 | 1.00 | 34.42 | X | O |
| ATOM | 6487 | C | SER | 35 | 83.105 | 34.548 | 23.761 | 1.00 | 35.95 | X | C |
| ATOM | 6488 | O | SER | 35 | 82.191 | 34.290 | 22.978 | 1.00 | 35.95 | X | O |
| ATOM | 6489 | N | TRP | 36 | 83.323 | 33.856 | 24.879 | 1.00 | 43.17 | X | N |
| ATOM | 6490 | CA | TRP | 36 | 82.457 | 32.758 | 25.309 | 1.00 | 43.17 | X | C |
| ATOM | 6491 | CB | TRP | 36 | 83.159 | 31.383 | 25.200 | 1.00 | 32.84 | X | C |
| ATOM | 6492 | CG | TRP | 36 | 83.355 | 30.875 | 23.782 | 1.00 | 32.84 | X | C |
| ATOM | 6493 | CD2 | TRP | 36 | 82.419 | 30.118 | 22.998 | 1.00 | 32.84 | X | C |
| ATOM | 6494 | CE2 | TRP | 36 | 82.982 | 29.957 | 21.711 | 1.00 | 32.84 | X | C |
| ATOM | 6495 | CE3 | TRP | 36 | 81.153 | 29.564 | 23.257 | 1.00 | 32.84 | X | C |
| ATOM | 6496 | CD1 | TRP | 36 | 84.419 | 31.124 | 22.962 | 1.00 | 32.84 | X | C |
| ATOM | 6497 | NE1 | TRP | 36 | 84.201 | 30.579 | 21.716 | 1.00 | 32.84 | X | N |

Fig. 19: A-90

```
ATOM   6498  CZ2 TRP    36      82.324  29.267  20.681  1.00  32.84      X    C
ATOM   6499  CZ3 TRP    36      80.495  28.877  22.228  1.00  32.84      X    C
ATOM   6500  CH2 TRP    36      81.086  28.738  20.957  1.00  32.84      X    C
ATOM   6501  C   TRP    36      82.056  33.022  26.764  1.00  43.17      X    C
ATOM   6502  O   TRP    36      82.908  33.298  27.615  1.00  43.17      X    O
ATOM   6503  N   VAL    37      80.751  32.958  27.026  1.00  29.19      X    N
ATOM   6504  CA  VAL    37      80.177  33.175  28.360  1.00  29.19      X    C
ATOM   6505  CB  VAL    37      79.213  34.419  28.353  1.00   8.00      X    C
ATOM   6506  CG1 VAL    37      78.350  34.467  29.621  1.00   8.00      X    C
ATOM   6507  CG2 VAL    37      80.026  35.689  28.240  1.00   8.00      X    C
ATOM   6508  C   VAL    37      79.412  31.907  28.760  1.00  29.19      X    C
ATOM   6509  O   VAL    37      78.629  31.381  27.971  1.00  29.19      X    O
ATOM   6510  N   ARG    38      79.651  31.415  29.974  1.00  61.80      X    N
ATOM   6511  CA  ARG    38      78.992  30.198  30.454  1.00  61.80      X    C
ATOM   6512  CB  ARG    38      80.036  29.167  30.899  1.00  27.50      X    C
ATOM   6513  CG  ARG    38      80.926  29.688  32.011  1.00  27.50      X    C
ATOM   6514  CD  ARG    38      81.370  28.603  32.965  1.00  27.50      X    C
ATOM   6515  NE  ARG    38      82.222  27.579  32.364  1.00  27.50      X    N
ATOM   6516  CZ  ARG    38      83.391  27.181  32.874  1.00  27.50      X    C
ATOM   6517  NH1 ARG    38      83.862  27.725  33.992  1.00  27.50      X    N
ATOM   6518  NH2 ARG    38      84.087  26.217  32.281  1.00  27.50      X    N
ATOM   6519  C   ARG    38      78.053  30.468  31.628  1.00  61.80      X    C
ATOM   6520  O   ARG    38      78.104  31.528  32.245  1.00  61.80      X    O
ATOM   6521  N   GLN    39      77.204  29.491  31.934  1.00  39.46      X    N
ATOM   6522  CA  GLN    39      76.269  29.597  33.049  1.00  39.46      X    C
ATOM   6523  CB  GLN    39      74.982  30.269  32.588  1.00  44.48      X    C
ATOM   6524  CG  GLN    39      73.997  30.530  33.708  1.00  44.48      X    C
ATOM   6525  CD  GLN    39      72.916  31.497  33.294  1.00  44.48      X    C
ATOM   6526  OE1 GLN    39      72.269  31.320  32.252  1.00  44.48      X    O
ATOM   6527  NE2 GLN    39      72.709  32.532  34.106  1.00  44.48      X    N
ATOM   6528  C   GLN    39      75.955  28.224  33.663  1.00  39.46      X    C
ATOM   6529  O   GLN    39      75.233  27.404  33.076  1.00  39.46      X    O
ATOM   6530  N   ALA    40      76.514  27.984  34.846  1.00  47.11      X    N
ATOM   6531  CA  ALA    40      76.324  26.727  35.558  1.00  47.11      X    C
ATOM   6532  CB  ALA    40      77.241  26.678  36.773  1.00  19.87      X    C
ATOM   6533  C   ALA    40      74.875  26.592  35.995  1.00  47.11      X    C
ATOM   6534  O   ALA    40      74.296  27.542  36.512  1.00  47.11      X    O
ATOM   6535  N   PRO    41      74.271  25.403  35.802  1.00  63.91      X    N
ATOM   6536  CD  PRO    41      74.879  24.157  35.299  1.00  66.56      X    C
ATOM   6537  CA  PRO    41      72.875  25.168  36.187  1.00  63.91      X    C
ATOM   6538  CB  PRO    41      72.793  23.649  36.244  1.00  66.56      X    C
ATOM   6539  CG  PRO    41      73.667  23.254  35.115  1.00  66.56      X    C
ATOM   6540  C   PRO    41      72.507  25.826  37.508  1.00  63.91      X    C
ATOM   6541  O   PRO    41      73.186  25.637  38.522  1.00  63.91      X    O
ATOM   6542  N   GLY    42      71.432  26.608  37.478  1.00  63.56      X    N
ATOM   6543  CA  GLY    42      70.979  27.297  38.671  1.00  63.56      X    C
ATOM   6544  C   GLY    42      71.963  28.342  39.165  1.00  63.56      X    C
ATOM   6545  O   GLY    42      71.920  28.732  40.334  1.00  63.56      X    O
ATOM   6546  N   LYS    43      72.846  28.793  38.276  1.00 103.79      X    N
ATOM   6547  CA  LYS    43      73.852  29.802  38.607  1.00 103.79      X    C
ATOM   6548  CB  LYS    43      75.248  29.168  38.641  1.00  95.84      X    C
ATOM   6549  CG  LYS    43      75.752  28.830  40.037  1.00  95.84      X    C
ATOM   6550  CD  LYS    43      74.840  27.853  40.755  1.00  95.84      X    C
ATOM   6551  CE  LYS    43      75.225  27.734  42.222  1.00  95.84      X    C
ATOM   6552  NZ  LYS    43      75.138  29.048  42.920  1.00  95.84      X    N
ATOM   6553  C   LYS    43      73.848  30.984  37.634  1.00 103.79      X    C
ATOM   6554  O   LYS    43      73.085  31.013  36.668  1.00 103.79      X    O
ATOM   6555  N   GLY    44      74.714  31.956  37.899  1.00  36.05      X    N
ATOM   6556  CA  GLY    44      74.796  33.131  37.055  1.00  36.05      X    C
ATOM   6557  C   GLY    44      75.710  33.025  35.845  1.00  36.05      X    C
ATOM   6558  O   GLY    44      76.150  31.931  35.477  1.00  36.05      X    O
ATOM   6559  N   LEU    45      76.003  34.186  35.249  1.00  24.14      X    N
ATOM   6560  CA  LEU    45      76.832  34.316  34.046  1.00  24.14      X    C
ATOM   6561  CB  LEU    45      76.343  35.504  33.214  1.00  15.59      X    C
ATOM   6562  CG  LEU    45      74.932  35.346  32.638  1.00  15.59      X    C
ATOM   6563  CD1 LEU    45      74.470  36.606  31.917  1.00  15.59      X    C
ATOM   6564  CD2 LEU    45      74.942  34.179  31.677  1.00  15.59      X    C
ATOM   6565  C   LEU    45      78.316  34.474  34.311  1.00  24.14      X    C
ATOM   6566  O   LEU    45      78.732  35.324  35.095  1.00  24.14      X    O
ATOM   6567  N   GLU    46      79.110  33.661  33.624  1.00  56.59      X    N
ATOM   6568  CA  GLU    46      80.557  33.686  33.774  1.00  56.59      X    C
ATOM   6569  CB  GLU    46      81.034  32.373  34.412  1.00  46.99      X    C
ATOM   6570  CG  GLU    46      82.536  32.308  34.666  1.00  46.99      X    C
```

Fig. 19: A-91

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 6571 | CD | GLU | 46 | 82.953 | 31.066 | 35.438 | 1.00 | 46.99 | X | C |
| ATOM | 6572 | OE1 | GLU | 46 | 82.642 | 29.952 | 34.970 | 1.00 | 46.99 | X | O |
| ATOM | 6573 | OE2 | GLU | 46 | 83.594 | 31.201 | 36.508 | 1.00 | 46.99 | X | O |
| ATOM | 6574 | C | GLU | 46 | 81.272 | 33.904 | 32.439 | 1.00 | 56.59 | X | C |
| ATOM | 6575 | O | GLU | 46 | 80.821 | 33.433 | 31.393 | 1.00 | 56.59 | X | O |
| ATOM | 6576 | N | TRP | 47 | 82.385 | 34.632 | 32.489 | 1.00 | 30.60 | X | N |
| ATOM | 6577 | CA | TRP | 47 | 83.188 | 34.910 | 31.300 | 1.00 | 30.60 | X | C |
| ATOM | 6578 | CB | TRP | 47 | 83.889 | 36.273 | 31.426 | 1.00 | 23.41 | X | C |
| ATOM | 6579 | CG | TRP | 47 | 84.944 | 36.481 | 30.385 | 1.00 | 23.41 | X | C |
| ATOM | 6580 | CD2 | TRP | 47 | 86.358 | 36.500 | 30.601 | 1.00 | 23.41 | X | C |
| ATOM | 6581 | CE2 | TRP | 47 | 86.971 | 36.591 | 29.328 | 1.00 | 23.41 | X | C |
| ATOM | 6582 | CE3 | TRP | 47 | 87.170 | 36.441 | 31.746 | 1.00 | 23.41 | X | C |
| ATOM | 6583 | CD1 | TRP | 47 | 84.759 | 36.570 | 29.031 | 1.00 | 23.41 | X | C |
| ATOM | 6584 | NE1 | TRP | 47 | 85.969 | 36.633 | 28.392 | 1.00 | 23.41 | X | N |
| ATOM | 6585 | CZ2 | TRP | 47 | 88.365 | 36.622 | 29.165 | 1.00 | 23.41 | X | C |
| ATOM | 6586 | CZ3 | TRP | 47 | 88.553 | 36.470 | 31.587 | 1.00 | 23.41 | X | C |
| ATOM | 6587 | CH2 | TRP | 47 | 89.137 | 36.560 | 30.304 | 1.00 | 23.41 | X | C |
| ATOM | 6588 | C | TRP | 47 | 84.231 | 33.810 | 31.153 | 1.00 | 30.60 | X | C |
| ATOM | 6589 | O | TRP | 47 | 84.965 | 33.516 | 32.097 | 1.00 | 30.60 | X | O |
| ATOM | 6590 | N | VAL | 48 | 84.317 | 33.219 | 29.967 | 1.00 | 24.17 | X | N |
| ATOM | 6591 | CA | VAL | 48 | 85.270 | 32.128 | 29.755 | 1.00 | 24.17 | X | C |
| ATOM | 6592 | CB | VAL | 48 | 84.589 | 30.924 | 29.011 | 1.00 | 22.03 | X | C |
| ATOM | 6593 | CG1 | VAL | 48 | 85.589 | 29.786 | 28.790 | 1.00 | 22.03 | X | C |
| ATOM | 6594 | CG2 | VAL | 48 | 83.408 | 30.436 | 29.805 | 1.00 | 22.03 | X | C |
| ATOM | 6595 | C | VAL | 48 | 86.550 | 32.490 | 29.006 | 1.00 | 24.17 | X | C |
| ATOM | 6596 | O | VAL | 48 | 87.640 | 32.477 | 29.579 | 1.00 | 24.17 | X | O |
| ATOM | 6597 | N | ALA | 49 | 86.407 | 32.800 | 27.724 | 1.00 | 21.43 | X | N |
| ATOM | 6598 | CA | ALA | 49 | 87.550 | 33.118 | 26.885 | 1.00 | 21.43 | X | C |
| ATOM | 6599 | CB | ALA | 49 | 87.953 | 31.884 | 26.094 | 1.00 | 38.48 | X | C |
| ATOM | 6600 | C | ALA | 49 | 87.228 | 34.257 | 25.934 | 1.00 | 21.43 | X | C |
| ATOM | 6601 | O | ALA | 49 | 86.066 | 34.661 | 25.825 | 1.00 | 21.43 | X | O |
| ATOM | 6602 | N | THR | 50 | 88.257 | 34.745 | 25.235 | 1.00 | 24.70 | X | N |
| ATOM | 6603 | CA | THR | 50 | 88.115 | 35.856 | 24.286 | 1.00 | 24.70 | X | C |
| ATOM | 6604 | CB | THR | 50 | 87.952 | 37.202 | 25.048 | 1.00 | 38.80 | X | C |
| ATOM | 6605 | OG1 | THR | 50 | 86.711 | 37.215 | 25.763 | 1.00 | 38.80 | X | O |
| ATOM | 6606 | CG2 | THR | 50 | 87.981 | 38.369 | 24.087 | 1.00 | 38.80 | X | C |
| ATOM | 6607 | C | THR | 50 | 89.298 | 36.039 | 23.324 | 1.00 | 24.70 | X | C |
| ATOM | 6608 | O | THR | 50 | 90.456 | 35.935 | 23.738 | 1.00 | 24.70 | X | O |
| ATOM | 6609 | N | ILE | 51 | 89.010 | 36.300 | 22.047 | 1.00 | 32.54 | X | N |
| ATOM | 6610 | CA | ILE | 51 | 90.075 | 36.599 | 21.074 | 1.00 | 32.54 | X | C |
| ATOM | 6611 | CB | ILE | 51 | 90.333 | 35.495 | 19.998 | 1.00 | 54.98 | X | C |
| ATOM | 6612 | CG2 | ILE | 51 | 90.567 | 34.178 | 20.661 | 1.00 | 54.98 | X | C |
| ATOM | 6613 | CG1 | ILE | 51 | 89.180 | 35.415 | 18.997 | 1.00 | 54.98 | X | C |
| ATOM | 6614 | CD1 | ILE | 51 | 87.893 | 34.921 | 19.582 | 1.00 | 54.98 | X | C |
| ATOM | 6615 | C | ILE | 51 | 89.674 | 37.865 | 20.335 | 1.00 | 32.54 | X | C |
| ATOM | 6616 | O | ILE | 51 | 88.516 | 38.024 | 19.937 | 1.00 | 32.54 | X | O |
| ATOM | 6617 | N | SER | 52 | 90.628 | 38.774 | 20.167 | 1.00 | 43.61 | X | N |
| ATOM | 6618 | CA | SER | 52 | 90.361 | 40.024 | 19.477 | 1.00 | 43.61 | X | C |
| ATOM | 6619 | CB | SER | 52 | 91.374 | 41.081 | 19.910 | 1.00 | 24.33 | X | C |
| ATOM | 6620 | OG | SER | 52 | 92.684 | 40.702 | 19.528 | 1.00 | 24.33 | X | O |
| ATOM | 6621 | C | SER | 52 | 90.450 | 39.789 | 17.973 | 1.00 | 43.61 | X | C |
| ATOM | 6622 | O | SER | 52 | 90.677 | 38.663 | 17.533 | 1.00 | 43.61 | X | O |
| ATOM | 6623 | N | GLY | 53 | 90.243 | 40.843 | 17.187 | 1.00 | 34.59 | X | N |
| ATOM | 6624 | CA | GLY | 53 | 90.336 | 40.707 | 15.747 | 1.00 | 34.59 | X | C |
| ATOM | 6625 | C | GLY | 53 | 91.800 | 40.559 | 15.381 | 1.00 | 34.59 | X | C |
| ATOM | 6626 | O | GLY | 53 | 92.152 | 40.020 | 14.332 | 1.00 | 34.59 | X | O |
| ATOM | 6627 | N | GLY | 54 | 92.658 | 41.047 | 16.266 | 1.00 | 29.30 | X | N |
| ATOM | 6628 | CA | GLY | 54 | 94.079 | 40.949 | 16.033 | 1.00 | 29.30 | X | C |
| ATOM | 6629 | C | GLY | 54 | 94.555 | 39.550 | 16.359 | 1.00 | 29.30 | X | C |
| ATOM | 6630 | O | GLY | 54 | 95.642 | 39.135 | 15.954 | 1.00 | 29.30 | X | O |
| ATOM | 6631 | N | GLY | 55 | 93.747 | 38.811 | 17.103 | 1.00 | 15.27 | X | N |
| ATOM | 6632 | CA | GLY | 55 | 94.139 | 37.465 | 17.437 | 1.00 | 15.27 | X | C |
| ATOM | 6633 | C | GLY | 55 | 94.596 | 37.254 | 18.867 | 1.00 | 15.27 | X | C |
| ATOM | 6634 | O | GLY | 55 | 94.878 | 36.105 | 19.231 | 1.00 | 15.27 | X | O |
| ATOM | 6635 | N | HIS | 56 | 94.676 | 38.319 | 19.675 | 1.00 | 13.76 | X | N |
| ATOM | 6636 | CA | HIS | 56 | 95.101 | 38.181 | 21.076 | 1.00 | 13.76 | X | C |
| ATOM | 6637 | CB | HIS | 56 | 95.268 | 39.543 | 21.741 | 1.00 | 60.58 | X | C |
| ATOM | 6638 | CG | HIS | 56 | 96.115 | 40.490 | 20.957 | 1.00 | 60.58 | X | C |
| ATOM | 6639 | CD2 | HIS | 56 | 97.417 | 40.838 | 21.087 | 1.00 | 60.58 | X | C |
| ATOM | 6640 | ND1 | HIS | 56 | 95.638 | 41.180 | 19.862 | 1.00 | 60.58 | X | N |
| ATOM | 6641 | CE1 | HIS | 56 | 96.611 | 41.913 | 19.351 | 1.00 | 60.58 | X | C |
| ATOM | 6642 | NE2 | HIS | 56 | 97.701 | 41.724 | 20.075 | 1.00 | 60.58 | X | N |
| ATOM | 6643 | C | HIS | 56 | 94.071 | 37.383 | 21.857 | 1.00 | 13.76 | X | C |

Fig. 19: A-92

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 6644 | O | HIS | 56 | 92.864 | 37.621 | 21.736 | 1.00 | 13.76 | X | O |
| ATOM | 6645 | N | THR | 57 | 94.529 | 36.438 | 22.671 | 1.00 | 20.05 | X | N |
| ATOM | 6646 | CA | THR | 57 | 93.583 | 35.632 | 23.436 | 1.00 | 20.05 | X | C |
| ATOM | 6647 | CB | THR | 57 | 93.759 | 34.123 | 23.096 | 1.00 | 15.53 | X | C |
| ATOM | 6648 | OG1 | THR | 57 | 95.015 | 33.651 | 23.587 | 1.00 | 15.53 | X | O |
| ATOM | 6649 | CG2 | THR | 57 | 93.734 | 33.929 | 21.593 | 1.00 | 15.53 | X | C |
| ATOM | 6650 | C | THR | 57 | 93.655 | 35.876 | 24.952 | 1.00 | 20.05 | X | C |
| ATOM | 6651 | O | THR | 57 | 94.716 | 36.142 | 25.512 | 1.00 | 20.05 | X | O |
| ATOM | 6652 | N | TYR | 58 | 92.500 | 35.808 | 25.603 | 1.00 | 19.06 | X | N |
| ATOM | 6653 | CA | TYR | 58 | 92.410 | 36.037 | 27.040 | 1.00 | 19.06 | X | C |
| ATOM | 6654 | CB | TYR | 58 | 91.829 | 37.428 | 27.304 | 1.00 | 22.48 | X | C |
| ATOM | 6655 | CG | TYR | 58 | 92.614 | 38.542 | 26.661 | 1.00 | 22.48 | X | C |
| ATOM | 6656 | CD1 | TYR | 58 | 93.565 | 39.252 | 27.384 | 1.00 | 22.48 | X | C |
| ATOM | 6657 | CE1 | TYR | 58 | 94.308 | 40.265 | 26.788 | 1.00 | 22.48 | X | C |
| ATOM | 6658 | CD2 | TYR | 58 | 92.423 | 38.871 | 25.316 | 1.00 | 22.48 | X | C |
| ATOM | 6659 | CE2 | TYR | 58 | 93.167 | 39.886 | 24.703 | 1.00 | 22.48 | X | C |
| ATOM | 6660 | CZ | TYR | 58 | 94.105 | 40.580 | 25.447 | 1.00 | 22.48 | X | C |
| ATOM | 6661 | OH | TYR | 58 | 94.828 | 41.611 | 24.876 | 1.00 | 22.48 | X | O |
| ATOM | 6662 | C | TYR | 58 | 91.513 | 34.973 | 27.656 | 1.00 | 19.06 | X | C |
| ATOM | 6663 | O | TYR | 58 | 90.442 | 34.660 | 27.123 | 1.00 | 19.06 | X | O |
| ATOM | 6664 | N | TYR | 59 | 91.945 | 34.437 | 28.792 | 1.00 | 29.06 | X | N |
| ATOM | 6665 | CA | TYR | 59 | 91.199 | 33.378 | 29.456 | 1.00 | 29.06 | X | C |
| ATOM | 6666 | CB | TYR | 59 | 91.988 | 32.080 | 29.371 | 1.00 | 21.37 | X | C |
| ATOM | 6667 | CG | TYR | 59 | 92.252 | 31.641 | 27.969 | 1.00 | 21.37 | X | C |
| ATOM | 6668 | CD1 | TYR | 59 | 91.352 | 30.813 | 27.303 | 1.00 | 21.37 | X | C |
| ATOM | 6669 | CE1 | TYR | 59 | 91.573 | 30.428 | 25.988 | 1.00 | 21.37 | X | C |
| ATOM | 6670 | CD2 | TYR | 59 | 93.382 | 32.076 | 27.286 | 1.00 | 21.37 | X | C |
| ATOM | 6671 | CE2 | TYR | 59 | 93.608 | 31.698 | 25.968 | 1.00 | 21.37 | X | C |
| ATOM | 6672 | CZ | TYR | 59 | 92.697 | 30.874 | 25.330 | 1.00 | 21.37 | X | C |
| ATOM | 6673 | OH | TYR | 59 | 92.897 | 30.495 | 24.027 | 1.00 | 21.37 | X | O |
| ATOM | 6674 | C | TYR | 59 | 90.857 | 33.605 | 30.910 | 1.00 | 29.06 | X | C |
| ATOM | 6675 | O | TYR | 59 | 91.575 | 34.287 | 31.648 | 1.00 | 29.06 | X | O |
| ATOM | 6676 | N | LEU | 60 | 89.745 | 33.002 | 31.308 | 1.00 | 26.45 | X | N |
| ATOM | 6677 | CA | LEU | 60 | 89.309 | 33.048 | 32.689 | 1.00 | 26.45 | X | C |
| ATOM | 6678 | CB | LEU | 60 | 87.927 | 32.397 | 32.826 | 1.00 | 24.21 | X | C |
| ATOM | 6679 | CG | LEU | 60 | 87.411 | 32.193 | 34.252 | 1.00 | 24.21 | X | C |
| ATOM | 6680 | CD1 | LEU | 60 | 87.173 | 33.538 | 34.911 | 1.00 | 24.21 | X | C |
| ATOM | 6681 | CD2 | LEU | 60 | 86.135 | 31.380 | 34.223 | 1.00 | 24.21 | X | C |
| ATOM | 6682 | C | LEU | 60 | 90.382 | 32.189 | 33.360 | 1.00 | 26.45 | X | C |
| ATOM | 6683 | O | LEU | 60 | 90.822 | 31.191 | 32.781 | 1.00 | 26.45 | X | O |
| ATOM | 6684 | N | ASP | 61 | 90.822 | 32.570 | 34.553 | 1.00 | 64.06 | X | N |
| ATOM | 6685 | CA | ASP | 61 | 91.865 | 31.810 | 35.240 | 1.00 | 64.06 | X | C |
| ATOM | 6686 | CB | ASP | 61 | 92.297 | 32.556 | 36.502 | 1.00 | 60.41 | X | C |
| ATOM | 6687 | CG | ASP | 61 | 92.984 | 33.865 | 36.183 | 1.00 | 60.41 | X | C |
| ATOM | 6688 | OD1 | ASP | 61 | 93.262 | 34.650 | 37.114 | 1.00 | 60.41 | X | O |
| ATOM | 6689 | OD2 | ASP | 61 | 93.250 | 34.106 | 34.986 | 1.00 | 60.41 | X | O |
| ATOM | 6690 | C | ASP | 61 | 91.477 | 30.371 | 35.576 | 1.00 | 64.06 | X | C |
| ATOM | 6691 | O | ASP | 61 | 92.337 | 29.503 | 35.701 | 1.00 | 64.06 | X | O |
| ATOM | 6692 | N | SER | 62 | 90.181 | 30.122 | 35.707 | 1.00 | 57.78 | X | N |
| ATOM | 6693 | CA | SER | 62 | 89.681 | 28.791 | 36.028 | 1.00 | 57.78 | X | C |
| ATOM | 6694 | CB | SER | 62 | 88.196 | 28.868 | 36.386 | 1.00 | 42.55 | X | C |
| ATOM | 6695 | OG | SER | 62 | 87.643 | 27.575 | 36.556 | 1.00 | 42.55 | X | O |
| ATOM | 6696 | C | SER | 62 | 89.872 | 27.787 | 34.894 | 1.00 | 57.78 | X | C |
| ATOM | 6697 | O | SER | 62 | 90.000 | 26.590 | 35.142 | 1.00 | 57.78 | X | O |
| ATOM | 6698 | N | VAL | 63 | 89.890 | 28.269 | 33.655 | 1.00 | 47.11 | X | N |
| ATOM | 6699 | CA | VAL | 63 | 90.047 | 27.383 | 32.504 | 1.00 | 47.11 | X | C |
| ATOM | 6700 | CB | VAL | 63 | 88.796 | 27.464 | 31.555 | 1.00 | 39.29 | X | C |
| ATOM | 6701 | CG1 | VAL | 63 | 87.513 | 27.472 | 32.375 | 1.00 | 39.29 | X | C |
| ATOM | 6702 | CG2 | VAL | 63 | 88.863 | 28.700 | 30.679 | 1.00 | 39.29 | X | C |
| ATOM | 6703 | C | VAL | 63 | 91.318 | 27.660 | 31.686 | 1.00 | 47.11 | X | C |
| ATOM | 6704 | O | VAL | 63 | 91.504 | 27.093 | 30.603 | 1.00 | 47.11 | X | O |
| ATOM | 6705 | N | LYS | 64 | 92.200 | 28.511 | 32.208 | 1.00 | 47.01 | X | N |
| ATOM | 6706 | CA | LYS | 64 | 93.424 | 28.843 | 31.483 | 1.00 | 47.01 | X | C |
| ATOM | 6707 | CB | LYS | 64 | 94.116 | 30.063 | 32.107 | 1.00 | 84.46 | X | C |
| ATOM | 6708 | CG | LYS | 64 | 95.038 | 30.797 | 31.135 | 1.00 | 84.46 | X | C |
| ATOM | 6709 | CD | LYS | 64 | 95.670 | 32.025 | 31.766 | 1.00 | 84.46 | X | C |
| ATOM | 6710 | CE | LYS | 64 | 96.370 | 32.907 | 30.725 | 1.00 | 84.46 | X | C |
| ATOM | 6711 | NZ | LYS | 64 | 95.419 | 33.654 | 29.833 | 1.00 | 84.46 | X | N |
| ATOM | 6712 | C | LYS | 64 | 94.388 | 27.666 | 31.441 | 1.00 | 47.01 | X | C |
| ATOM | 6713 | O | LYS | 64 | 94.757 | 27.113 | 32.479 | 1.00 | 47.01 | X | O |
| ATOM | 6714 | N | GLY | 65 | 94.795 | 27.289 | 30.231 | 1.00 | 35.35 | X | N |
| ATOM | 6715 | CA | GLY | 65 | 95.704 | 26.167 | 30.073 | 1.00 | 35.35 | X | C |
| ATOM | 6716 | C | GLY | 65 | 94.953 | 24.919 | 29.652 | 1.00 | 35.35 | X | C |

Fig. 19: A-93

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 6717 | O | GLY | 65 | 95.547 | 23.945 | 29.195 | 1.00 | 35.35 | X | O |
| ATOM | 6718 | N | ARG | 66 | 93.634 | 24.956 | 29.809 | 1.00 | 33.32 | X | N |
| ATOM | 6719 | CA | ARG | 66 | 92.791 | 23.833 | 29.450 | 1.00 | 33.32 | X | C |
| ATOM | 6720 | CB | ARG | 66 | 91.881 | 23.470 | 30.616 | 1.00 | 43.17 | X | C |
| ATOM | 6721 | CG | ARG | 66 | 92.594 | 23.386 | 31.958 | 1.00 | 43.17 | X | C |
| ATOM | 6722 | CD | ARG | 66 | 91.684 | 22.813 | 33.050 | 1.00 | 43.17 | X | C |
| ATOM | 6723 | NE | ARG | 66 | 90.548 | 23.679 | 33.367 | 1.00 | 43.17 | X | N |
| ATOM | 6724 | CZ | ARG | 66 | 89.277 | 23.296 | 33.305 | 1.00 | 43.17 | X | C |
| ATOM | 6725 | NH1 | ARG | 66 | 88.973 | 22.061 | 32.932 | 1.00 | 43.17 | X | N |
| ATOM | 6726 | NH2 | ARG | 66 | 88.309 | 24.144 | 33.630 | 1.00 | 43.17 | X | N |
| ATOM | 6727 | C | ARG | 66 | 91.945 | 24.169 | 28.232 | 1.00 | 33.32 | X | C |
| ATOM | 6728 | O | ARG | 66 | 91.775 | 23.336 | 27.346 | 1.00 | 33.32 | X | O |
| ATOM | 6729 | N | PHE | 67 | 91.411 | 25.389 | 28.191 | 1.00 | 33.69 | X | N |
| ATOM | 6730 | CA | PHE | 67 | 90.567 | 25.834 | 27.074 | 1.00 | 33.69 | X | C |
| ATOM | 6731 | CB | PHE | 67 | 89.444 | 26.750 | 27.587 | 1.00 | 42.44 | X | C |
| ATOM | 6732 | CG | PHE | 67 | 88.346 | 26.030 | 28.330 | 1.00 | 42.44 | X | C |
| ATOM | 6733 | CD1 | PHE | 67 | 88.573 | 24.802 | 28.943 | 1.00 | 42.44 | X | C |
| ATOM | 6734 | CD2 | PHE | 67 | 87.074 | 26.594 | 28.426 | 1.00 | 42.44 | X | C |
| ATOM | 6735 | CE1 | PHE | 67 | 87.547 | 24.145 | 29.637 | 1.00 | 42.44 | X | C |
| ATOM | 6736 | CE2 | PHE | 67 | 86.038 | 25.940 | 29.122 | 1.00 | 42.44 | X | C |
| ATOM | 6737 | CZ | PHE | 67 | 86.278 | 24.717 | 29.724 | 1.00 | 42.44 | X | C |
| ATOM | 6738 | C | PHE | 67 | 91.393 | 26.578 | 26.027 | 1.00 | 33.69 | X | C |
| ATOM | 6739 | O | PHE | 67 | 92.405 | 27.194 | 26.344 | 1.00 | 33.69 | X | O |
| ATOM | 6740 | N | THR | 68 | 90.949 | 26.526 | 24.779 | 1.00 | 56.59 | X | N |
| ATOM | 6741 | CA | THR | 68 | 91.646 | 27.201 | 23.689 | 1.00 | 56.59 | X | C |
| ATOM | 6742 | CB | THR | 68 | 92.454 | 26.193 | 22.846 | 1.00 | 46.98 | X | C |
| ATOM | 6743 | OG1 | THR | 68 | 93.611 | 25.781 | 23.578 | 1.00 | 46.98 | X | O |
| ATOM | 6744 | CG2 | THR | 68 | 92.870 | 26.808 | 21.512 | 1.00 | 46.98 | X | C |
| ATOM | 6745 | C | THR | 68 | 90.661 | 27.913 | 22.768 | 1.00 | 56.59 | X | C |
| ATOM | 6746 | O | THR | 68 | 89.899 | 27.270 | 22.047 | 1.00 | 56.59 | X | O |
| ATOM | 6747 | N | ILE | 69 | 90.672 | 29.239 | 22.781 | 1.00 | 20.15 | X | N |
| ATOM | 6748 | CA | ILE | 69 | 89.760 | 29.975 | 21.918 | 1.00 | 20.15 | X | C |
| ATOM | 6749 | CB | ILE | 69 | 89.287 | 31.289 | 22.607 | 1.00 | 31.46 | X | C |
| ATOM | 6750 | CG2 | ILE | 69 | 90.480 | 32.153 | 22.953 | 1.00 | 31.46 | X | C |
| ATOM | 6751 | CG1 | ILE | 69 | 88.283 | 32.028 | 21.722 | 1.00 | 31.46 | X | C |
| ATOM | 6752 | CD1 | ILE | 69 | 87.574 | 33.159 | 22.446 | 1.00 | 31.46 | X | C |
| ATOM | 6753 | C | ILE | 69 | 90.464 | 30.262 | 20.591 | 1.00 | 20.15 | X | C |
| ATOM | 6754 | O | ILE | 69 | 91.672 | 30.481 | 20.559 | 1.00 | 20.15 | X | O |
| ATOM | 6755 | N | SER | 70 | 89.724 | 30.223 | 19.489 | 1.00 | 21.14 | X | N |
| ATOM | 6756 | CA | SER | 70 | 90.319 | 30.482 | 18.182 | 1.00 | 21.14 | X | C |
| ATOM | 6757 | CB | SER | 70 | 91.105 | 29.263 | 17.693 | 1.00 | 37.41 | X | C |
| ATOM | 6758 | OG | SER | 70 | 90.228 | 28.236 | 17.253 | 1.00 | 37.41 | X | O |
| ATOM | 6759 | C | SER | 70 | 89.242 | 30.824 | 17.163 | 1.00 | 21.14 | X | C |
| ATOM | 6760 | O | SER | 70 | 88.045 | 30.637 | 17.413 | 1.00 | 21.14 | X | O |
| ATOM | 6761 | N | ARG | 71 | 89.673 | 31.322 | 16.009 | 1.00 | 30.73 | X | N |
| ATOM | 6762 | CA | ARG | 71 | 88.734 | 31.687 | 14.966 | 1.00 | 30.73 | X | C |
| ATOM | 6763 | CB | ARG | 71 | 88.369 | 33.178 | 15.073 | 1.00 | 24.51 | X | C |
| ATOM | 6764 | CG | ARG | 71 | 89.546 | 34.139 | 14.901 | 1.00 | 24.51 | X | C |
| ATOM | 6765 | CD | ARG | 71 | 89.071 | 35.503 | 14.453 | 1.00 | 24.51 | X | C |
| ATOM | 6766 | NE | ARG | 71 | 88.464 | 36.278 | 15.534 | 1.00 | 24.51 | X | N |
| ATOM | 6767 | CZ | ARG | 71 | 87.604 | 37.283 | 15.351 | 1.00 | 24.51 | X | C |
| ATOM | 6768 | NH1 | ARG | 71 | 87.229 | 37.643 | 14.131 | 1.00 | 24.51 | X | N |
| ATOM | 6769 | NH2 | ARG | 71 | 87.132 | 37.948 | 16.391 | 1.00 | 24.51 | X | N |
| ATOM | 6770 | C | ARG | 71 | 89.259 | 31.393 | 13.560 | 1.00 | 30.73 | X | C |
| ATOM | 6771 | O | ARG | 71 | 90.464 | 31.415 | 13.301 | 1.00 | 30.73 | X | O |
| ATOM | 6772 | N | ASP | 72 | 88.326 | 31.106 | 12.663 | 1.00 | 55.72 | X | N |
| ATOM | 6773 | CA | ASP | 72 | 88.619 | 30.836 | 11.268 | 1.00 | 55.72 | X | C |
| ATOM | 6774 | CB | ASP | 72 | 88.219 | 29.405 | 10.902 | 1.00 | 83.09 | X | C |
| ATOM | 6775 | CG | ASP | 72 | 88.255 | 29.153 | 9.409 | 1.00 | 83.09 | X | C |
| ATOM | 6776 | OD1 | ASP | 72 | 89.282 | 29.466 | 8.773 | 1.00 | 83.09 | X | O |
| ATOM | 6777 | OD2 | ASP | 72 | 87.256 | 28.637 | 8.870 | 1.00 | 83.09 | X | O |
| ATOM | 6778 | C | ASP | 72 | 87.749 | 31.837 | 10.528 | 1.00 | 55.72 | X | C |
| ATOM | 6779 | O | ASP | 72 | 86.613 | 31.539 | 10.162 | 1.00 | 55.72 | X | O |
| ATOM | 6780 | N | ASN | 73 | 88.284 | 33.036 | 10.340 | 1.00 | 57.89 | X | N |
| ATOM | 6781 | CA | ASN | 73 | 87.552 | 34.098 | 9.673 | 1.00 | 57.89 | X | C |
| ATOM | 6782 | CB | ASN | 73 | 88.426 | 35.345 | 9.558 | 1.00 | 43.96 | X | C |
| ATOM | 6783 | CG | ASN | 73 | 88.777 | 35.928 | 10.912 | 1.00 | 43.96 | X | C |
| ATOM | 6784 | OD1 | ASN | 73 | 88.021 | 35.794 | 11.879 | 1.00 | 43.96 | X | O |
| ATOM | 6785 | ND2 | ASN | 73 | 89.919 | 36.593 | 10.986 | 1.00 | 43.96 | X | N |
| ATOM | 6786 | C | ASN | 73 | 87.020 | 33.715 | 8.306 | 1.00 | 57.89 | X | C |
| ATOM | 6787 | O | ASN | 73 | 85.949 | 34.173 | 7.903 | 1.00 | 57.89 | X | O |
| ATOM | 6788 | N | SER | 74 | 87.756 | 32.870 | 7.594 | 1.00 | 50.09 | X | N |
| ATOM | 6789 | CA | SER | 74 | 87.324 | 32.451 | 6.268 | 1.00 | 50.09 | X | C |

# Fig. 19: A-94

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 6790 | CB | SER | 74 | 88.277 | 31.398 | 5.705 | 1.00 | 34.87 | X | C |
| ATOM | 6791 | OG | SER | 74 | 88.179 | 30.197 | 6.441 | 1.00 | 34.87 | X | O |
| ATOM | 6792 | C | SER | 74 | 85.910 | 31.880 | 6.303 | 1.00 | 50.09 | X | C |
| ATOM | 6793 | O | SER | 74 | 85.141 | 32.050 | 5.356 | 1.00 | 50.09 | X | O |
| ATOM | 6794 | N | LYS | 75 | 85.572 | 31.209 | 7.400 | 1.00 | 50.16 | X | N |
| ATOM | 6795 | CA | LYS | 75 | 84.257 | 30.597 | 7.551 | 1.00 | 50.16 | X | C |
| ATOM | 6796 | CB | LYS | 75 | 84.418 | 29.097 | 7.814 | 1.00 | 60.89 | X | C |
| ATOM | 6797 | CG | LYS | 75 | 85.206 | 28.372 | 6.729 | 1.00 | 60.89 | X | C |
| ATOM | 6798 | CD | LYS | 75 | 85.356 | 26.884 | 7.009 | 1.00 | 60.89 | X | C |
| ATOM | 6799 | CE | LYS | 75 | 86.046 | 26.195 | 5.840 | 1.00 | 60.89 | X | C |
| ATOM | 6800 | NZ | LYS | 75 | 85.341 | 26.459 | 4.551 | 1.00 | 60.89 | X | N |
| ATOM | 6801 | C | LYS | 75 | 83.423 | 31.226 | 8.663 | 1.00 | 50.16 | X | C |
| ATOM | 6802 | O | LYS | 75 | 82.470 | 30.618 | 9.142 | 1.00 | 50.16 | X | O |
| ATOM | 6803 | N | ASN | 76 | 83.786 | 32.441 | 9.066 | 1.00 | 54.49 | X | N |
| ATOM | 6804 | CA | ASN | 76 | 83.075 | 33.165 | 10.117 | 1.00 | 54.49 | X | C |
| ATOM | 6805 | CB | ASN | 76 | 81.812 | 33.818 | 9.559 | 1.00 | 41.29 | X | C |
| ATOM | 6806 | CG | ASN | 76 | 82.116 | 34.956 | 8.620 | 1.00 | 41.29 | X | C |
| ATOM | 6807 | OD1 | ASN | 76 | 81.399 | 35.956 | 8.592 | 1.00 | 41.29 | X | O |
| ATOM | 6808 | ND2 | ASN | 76 | 83.181 | 34.812 | 7.839 | 1.00 | 41.29 | X | N |
| ATOM | 6809 | C | ASN | 76 | 82.684 | 32.285 | 11.286 | 1.00 | 54.49 | X | C |
| ATOM | 6810 | O | ASN | 76 | 81.523 | 32.278 | 11.706 | 1.00 | 54.49 | X | O |
| ATOM | 6811 | N | THR | 77 | 83.645 | 31.550 | 11.827 | 1.00 | 48.88 | X | N |
| ATOM | 6812 | CA | THR | 77 | 83.325 | 30.675 | 12.938 | 1.00 | 48.88 | X | C |
| ATOM | 6813 | CB | THR | 77 | 83.321 | 29.215 | 12.481 | 1.00 | 67.62 | X | C |
| ATOM | 6814 | OG1 | THR | 77 | 82.318 | 29.048 | 11.469 | 1.00 | 67.62 | X | O |
| ATOM | 6815 | CG2 | THR | 77 | 83.028 | 28.284 | 13.653 | 1.00 | 67.62 | X | C |
| ATOM | 6816 | C | THR | 77 | 84.245 | 30.817 | 14.132 | 1.00 | 48.88 | X | C |
| ATOM | 6817 | O | THR | 77 | 85.463 | 30.858 | 13.990 | 1.00 | 48.88 | X | O |
| ATOM | 6818 | N | LEU | 78 | 83.641 | 30.900 | 15.313 | 1.00 | 25.08 | X | N |
| ATOM | 6819 | CA | LEU | 78 | 84.387 | 31.014 | 16.562 | 1.00 | 25.08 | X | C |
| ATOM | 6820 | CB | LEU | 78 | 83.739 | 32.047 | 17.488 | 1.00 | 24.57 | X | C |
| ATOM | 6821 | CG | LEU | 78 | 84.362 | 32.022 | 18.881 | 1.00 | 24.57 | X | C |
| ATOM | 6822 | CD1 | LEU | 78 | 85.757 | 32.625 | 18.789 | 1.00 | 24.57 | X | C |
| ATOM | 6823 | CD2 | LEU | 78 | 83.507 | 32.770 | 19.868 | 1.00 | 24.57 | X | C |
| ATOM | 6824 | C | LEU | 78 | 84.370 | 29.653 | 17.250 | 1.00 | 25.08 | X | C |
| ATOM | 6825 | O | LEU | 78 | 83.312 | 29.041 | 17.389 | 1.00 | 25.08 | X | O |
| ATOM | 6826 | N | TYR | 79 | 85.530 | 29.179 | 17.687 | 1.00 | 41.94 | X | N |
| ATOM | 6827 | CA | TYR | 79 | 85.595 | 27.880 | 18.344 | 1.00 | 41.94 | X | C |
| ATOM | 6828 | CB | TYR | 79 | 86.608 | 26.963 | 17.657 | 1.00 | 47.62 | X | C |
| ATOM | 6829 | CG | TYR | 79 | 86.328 | 26.619 | 16.226 | 1.00 | 47.62 | X | C |
| ATOM | 6830 | CD1 | TYR | 79 | 85.264 | 25.794 | 15.887 | 1.00 | 47.62 | X | C |
| ATOM | 6831 | CE1 | TYR | 79 | 85.008 | 25.460 | 14.559 | 1.00 | 47.62 | X | C |
| ATOM | 6832 | CD2 | TYR | 79 | 87.139 | 27.108 | 15.207 | 1.00 | 47.62 | X | C |
| ATOM | 6833 | CE2 | TYR | 79 | 86.896 | 26.784 | 13.878 | 1.00 | 47.62 | X | C |
| ATOM | 6834 | CZ | TYR | 79 | 85.826 | 25.959 | 13.559 | 1.00 | 47.62 | X | C |
| ATOM | 6835 | OH | TYR | 79 | 85.564 | 25.640 | 12.245 | 1.00 | 47.62 | X | O |
| ATOM | 6836 | C | TYR | 79 | 86.043 | 27.991 | 19.779 | 1.00 | 41.94 | X | C |
| ATOM | 6837 | O | TYR | 79 | 86.890 | 28.824 | 20.100 | 1.00 | 41.94 | X | O |
| ATOM | 6838 | N | LEU | 80 | 85.470 | 27.160 | 20.642 | 1.00 | 19.15 | X | N |
| ATOM | 6839 | CA | LEU | 80 | 85.917 | 27.110 | 22.022 | 1.00 | 19.15 | X | C |
| ATOM | 6840 | CB | LEU | 80 | 84.809 | 27.382 | 23.047 | 1.00 | 21.08 | X | C |
| ATOM | 6841 | CG | LEU | 80 | 85.271 | 27.127 | 24.510 | 1.00 | 21.08 | X | C |
| ATOM | 6842 | CD1 | LEU | 80 | 86.500 | 27.981 | 24.840 | 1.00 | 21.08 | X | C |
| ATOM | 6843 | CD2 | LEU | 80 | 84.142 | 27.412 | 25.503 | 1.00 | 21.08 | X | C |
| ATOM | 6844 | C | LEU | 80 | 86.342 | 25.671 | 22.129 | 1.00 | 19.15 | X | C |
| ATOM | 6845 | O | LEU | 80 | 85.517 | 24.769 | 21.941 | 1.00 | 19.15 | X | O |
| ATOM | 6846 | N | GLN | 81 | 87.631 | 25.455 | 22.395 | 1.00 | 31.28 | X | N |
| ATOM | 6847 | CA | GLN | 81 | 88.193 | 24.111 | 22.530 | 1.00 | 31.28 | X | C |
| ATOM | 6848 | CB | GLN | 81 | 89.497 | 24.015 | 21.738 | 1.00 | 68.87 | X | C |
| ATOM | 6849 | CG | GLN | 81 | 90.141 | 22.647 | 21.783 | 1.00 | 68.87 | X | C |
| ATOM | 6850 | CD | GLN | 81 | 89.318 | 21.580 | 21.075 | 1.00 | 68.87 | X | C |
| ATOM | 6851 | OE1 | GLN | 81 | 89.101 | 21.648 | 19.864 | 1.00 | 68.87 | X | O |
| ATOM | 6852 | NE2 | GLN | 81 | 88.857 | 20.588 | 21.831 | 1.00 | 68.87 | X | N |
| ATOM | 6853 | C | GLN | 81 | 88.448 | 23.775 | 24.001 | 1.00 | 31.28 | X | C |
| ATOM | 6854 | O | GLN | 81 | 89.402 | 24.260 | 24.604 | 1.00 | 31.28 | X | O |
| ATOM | 6855 | N | MET | 82 | 87.589 | 22.935 | 24.569 | 1.00 | 32.50 | X | N |
| ATOM | 6856 | CA | MET | 82 | 87.701 | 22.541 | 25.975 | 1.00 | 32.50 | X | C |
| ATOM | 6857 | CB | MET | 82 | 86.297 | 22.429 | 26.589 | 1.00 | 41.50 | X | C |
| ATOM | 6858 | CG | MET | 82 | 85.537 | 23.752 | 26.653 | 1.00 | 41.50 | X | C |
| ATOM | 6859 | SD | MET | 82 | 83.790 | 23.594 | 27.062 | 1.00 | 41.50 | X | S |
| ATOM | 6860 | CE | MET | 82 | 83.088 | 23.391 | 25.452 | 1.00 | 41.50 | X | C |
| ATOM | 6861 | C | MET | 82 | 88.463 | 21.230 | 26.188 | 1.00 | 32.50 | X | C |
| ATOM | 6862 | O | MET | 82 | 88.239 | 20.250 | 25.487 | 1.00 | 32.50 | X | O |

Fig. 19: A-95

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 6863 | N | ASN | 83 | 89.369 | 21.224 | 27.160 | 1.00 | 43.69 | X | N |
| ATOM | 6864 | CA | ASN | 83 | 90.155 | 20.032 | 27.459 | 1.00 | 43.69 | X | C |
| ATOM | 6865 | CB | ASN | 83 | 91.574 | 20.157 | 26.883 | 1.00 | 34.50 | X | C |
| ATOM | 6866 | CG | ASN | 83 | 91.574 | 20.391 | 25.383 | 1.00 | 34.50 | X | C |
| ATOM | 6867 | OD1 | ASN | 83 | 90.920 | 19.670 | 24.636 | 1.00 | 34.50 | X | O |
| ATOM | 6868 | ND2 | ASN | 83 | 92.313 | 21.401 | 24.937 | 1.00 | 34.50 | X | N |
| ATOM | 6869 | C | ASN | 83 | 90.225 | 19.855 | 28.967 | 1.00 | 43.69 | X | C |
| ATOM | 6870 | O | ASN | 83 | 90.054 | 20.822 | 29.705 | 1.00 | 43.69 | X | O |
| ATOM | 6871 | N | SER | 84 | 90.480 | 18.625 | 29.416 | 1.00 | 47.01 | X | N |
| ATOM | 6872 | CA | SER | 84 | 90.560 | 18.322 | 30.843 | 1.00 | 47.01 | X | C |
| ATOM | 6873 | CB | SER | 84 | 91.748 | 19.045 | 31.482 | 1.00 | 36.84 | X | C |
| ATOM | 6874 | OG | SER | 84 | 92.963 | 18.623 | 30.892 | 1.00 | 36.84 | X | O |
| ATOM | 6875 | C | SER | 84 | 89.270 | 18.757 | 31.516 | 1.00 | 47.01 | X | C |
| ATOM | 6876 | O | SER | 84 | 89.272 | 19.261 | 32.644 | 1.00 | 47.01 | X | O |
| ATOM | 6877 | N | LEU | 85 | 88.170 | 18.548 | 30.804 | 1.00 | 35.88 | X | N |
| ATOM | 6878 | CA | LEU | 85 | 86.842 | 18.920 | 31.273 | 1.00 | 35.88 | X | C |
| ATOM | 6879 | CB | LEU | 85 | 85.800 | 18.466 | 30.250 | 1.00 | 45.16 | X | C |
| ATOM | 6880 | CG | LEU | 85 | 85.854 | 19.211 | 28.921 | 1.00 | 45.16 | X | C |
| ATOM | 6881 | CD1 | LEU | 85 | 84.875 | 18.608 | 27.936 | 1.00 | 45.16 | X | C |
| ATOM | 6882 | CD2 | LEU | 85 | 85.536 | 20.672 | 29.178 | 1.00 | 45.16 | X | C |
| ATOM | 6883 | C | LEU | 85 | 86.450 | 18.396 | 32.652 | 1.00 | 35.88 | X | C |
| ATOM | 6884 | O | LEU | 85 | 86.175 | 17.208 | 32.818 | 1.00 | 35.88 | X | O |
| ATOM | 6885 | N | ARG | 86 | 86.415 | 19.290 | 33.636 | 1.00 | 55.90 | X | N |
| ATOM | 6886 | CA | ARG | 86 | 86.022 | 18.907 | 34.985 | 1.00 | 55.90 | X | C |
| ATOM | 6887 | CB | ARG | 86 | 86.606 | 19.864 | 36.023 | 1.00 | 50.18 | X | C |
| ATOM | 6888 | CG | ARG | 86 | 88.108 | 20.015 | 35.994 | 1.00 | 50.18 | X | C |
| ATOM | 6889 | CD | ARG | 86 | 88.620 | 20.357 | 37.385 | 1.00 | 50.18 | X | C |
| ATOM | 6890 | NE | ARG | 86 | 89.970 | 20.904 | 37.355 | 1.00 | 50.18 | X | N |
| ATOM | 6891 | CZ | ARG | 86 | 90.256 | 22.185 | 37.133 | 1.00 | 50.18 | X | C |
| ATOM | 6892 | NH1 | ARG | 86 | 89.280 | 23.066 | 36.926 | 1.00 | 50.18 | X | N |
| ATOM | 6893 | NH2 | ARG | 86 | 91.524 | 22.587 | 37.109 | 1.00 | 50.18 | X | N |
| ATOM | 6894 | C | ARG | 86 | 84.501 | 18.954 | 35.069 | 1.00 | 55.90 | X | C |
| ATOM | 6895 | O | ARG | 86 | 83.818 | 19.086 | 34.055 | 1.00 | 55.90 | X | O |
| ATOM | 6896 | N | ALA | 87 | 83.974 | 18.856 | 36.282 | 1.00 | 39.09 | X | N |
| ATOM | 6897 | CA | ALA | 87 | 82.533 | 18.893 | 36.485 | 1.00 | 39.09 | X | C |
| ATOM | 6898 | CB | ALA | 87 | 82.164 | 18.133 | 37.750 | 1.00 | 69.79 | X | C |
| ATOM | 6899 | C | ALA | 87 | 82.028 | 20.325 | 36.578 | 1.00 | 39.09 | X | C |
| ATOM | 6900 | O | ALA | 87 | 80.885 | 20.607 | 36.219 | 1.00 | 39.09 | X | O |
| ATOM | 6901 | N | GLU | 88 | 82.876 | 21.228 | 37.066 | 1.00 | 49.44 | X | N |
| ATOM | 6902 | CA | GLU | 88 | 82.492 | 22.628 | 37.197 | 1.00 | 49.44 | X | C |
| ATOM | 6903 | CB | GLU | 88 | 83.586 | 23.435 | 37.899 | 1.00 | 57.40 | X | C |
| ATOM | 6904 | CG | GLU | 88 | 84.189 | 22.765 | 39.107 | 1.00 | 57.40 | X | C |
| ATOM | 6905 | CD | GLU | 88 | 85.178 | 21.691 | 38.724 | 1.00 | 57.40 | X | C |
| ATOM | 6906 | OE1 | GLU | 88 | 86.227 | 22.035 | 38.146 | 1.00 | 57.40 | X | O |
| ATOM | 6907 | OE2 | GLU | 88 | 84.906 | 20.504 | 38.993 | 1.00 | 57.40 | X | O |
| ATOM | 6908 | C | GLU | 88 | 82.242 | 23.242 | 35.824 | 1.00 | 49.44 | X | C |
| ATOM | 6909 | O | GLU | 88 | 81.474 | 24.195 | 35.687 | 1.00 | 49.44 | X | O |
| ATOM | 6910 | N | ASP | 89 | 82.892 | 22.698 | 34.803 | 1.00 | 49.12 | X | N |
| ATOM | 6911 | CA | ASP | 89 | 82.720 | 23.229 | 33.464 | 1.00 | 49.12 | X | C |
| ATOM | 6912 | CB | ASP | 89 | 83.818 | 22.698 | 32.549 | 1.00 | 52.75 | X | C |
| ATOM | 6913 | CG | ASP | 89 | 85.194 | 22.903 | 33.124 | 1.00 | 52.75 | X | C |
| ATOM | 6914 | OD1 | ASP | 89 | 85.430 | 23.960 | 33.752 | 1.00 | 52.75 | X | O |
| ATOM | 6915 | OD2 | ASP | 89 | 86.043 | 22.011 | 32.936 | 1.00 | 52.75 | X | O |
| ATOM | 6916 | C | ASP | 89 | 81.348 | 22.914 | 32.871 | 1.00 | 49.12 | X | C |
| ATOM | 6917 | O | ASP | 89 | 80.981 | 23.459 | 31.834 | 1.00 | 49.12 | X | O |
| ATOM | 6918 | N | THR | 90 | 80.590 | 22.034 | 33.517 | 1.00 | 33.14 | X | N |
| ATOM | 6919 | CA | THR | 90 | 79.265 | 21.686 | 33.012 | 1.00 | 33.14 | X | C |
| ATOM | 6920 | CB | THR | 90 | 78.652 | 20.480 | 33.766 | 1.00 | 40.77 | X | C |
| ATOM | 6921 | OG1 | THR | 90 | 78.585 | 20.770 | 35.162 | 1.00 | 40.77 | X | O |
| ATOM | 6922 | CG2 | THR | 90 | 79.498 | 19.257 | 33.590 | 1.00 | 40.77 | X | C |
| ATOM | 6923 | C | THR | 90 | 78.361 | 22.899 | 33.174 | 1.00 | 33.14 | X | C |
| ATOM | 6924 | O | THR | 90 | 78.260 | 23.486 | 34.263 | 1.00 | 33.14 | X | O |
| ATOM | 6925 | N | ALA | 91 | 77.718 | 23.276 | 32.076 | 1.00 | 55.37 | X | N |
| ATOM | 6926 | CA | ALA | 91 | 76.832 | 24.428 | 32.058 | 1.00 | 55.37 | X | C |
| ATOM | 6927 | CB | ALA | 91 | 77.527 | 25.625 | 32.692 | 1.00 | 7.95 | X | C |
| ATOM | 6928 | C | ALA | 91 | 76.504 | 24.732 | 30.609 | 1.00 | 55.37 | X | C |
| ATOM | 6929 | O | ALA | 91 | 77.073 | 24.128 | 29.698 | 1.00 | 55.37 | X | O |
| ATOM | 6930 | N | VAL | 92 | 75.579 | 25.656 | 30.387 | 1.00 | 44.83 | X | N |
| ATOM | 6931 | CA | VAL | 92 | 75.243 | 26.017 | 29.021 | 1.00 | 44.83 | X | C |
| ATOM | 6932 | CB | VAL | 92 | 73.747 | 26.429 | 28.878 | 1.00 | 41.51 | X | C |
| ATOM | 6933 | CG1 | VAL | 92 | 73.210 | 26.967 | 30.198 | 1.00 | 41.51 | X | C |
| ATOM | 6934 | CG2 | VAL | 92 | 73.596 | 27.460 | 27.769 | 1.00 | 41.51 | X | C |
| ATOM | 6935 | C | VAL | 92 | 76.182 | 27.145 | 28.591 | 1.00 | 44.83 | X | C |

Fig. 19: A-96

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 6936 | O | VAL | 92 | 76.446 | 28.085 | 29.354 | 1.00 | 44.83 | X | O |
| ATOM | 6937 | N | TYR | 93 | 76.701 | 27.019 | 27.371 | 1.00 | 51.76 | X | N |
| ATOM | 6938 | CA | TYR | 93 | 77.642 | 27.978 | 26.811 | 1.00 | 51.76 | X | C |
| ATOM | 6939 | CB | TYR | 93 | 78.838 | 27.241 | 26.227 | 1.00 | 15.58 | X | C |
| ATOM | 6940 | CG | TYR | 93 | 79.743 | 26.693 | 27.287 | 1.00 | 15.58 | X | C |
| ATOM | 6941 | CD1 | TYR | 93 | 79.520 | 25.443 | 27.841 | 1.00 | 15.58 | X | C |
| ATOM | 6942 | CE1 | TYR | 93 | 80.339 | 24.959 | 28.860 | 1.00 | 15.58 | X | C |
| ATOM | 6943 | CD2 | TYR | 93 | 80.802 | 27.454 | 27.777 | 1.00 | 15.58 | X | C |
| ATOM | 6944 | CE2 | TYR | 93 | 81.618 | 26.983 | 28.797 | 1.00 | 15.58 | X | C |
| ATOM | 6945 | CZ | TYR | 93 | 81.384 | 25.735 | 29.328 | 1.00 | 15.58 | X | C |
| ATOM | 6946 | OH | TYR | 93 | 82.223 | 25.253 | 30.297 | 1.00 | 15.58 | X | O |
| ATOM | 6947 | C | TYR | 93 | 77.091 | 28.908 | 25.757 | 1.00 | 51.76 | X | C |
| ATOM | 6948 | O | TYR | 93 | 76.223 | 28.534 | 24.972 | 1.00 | 51.76 | X | O |
| ATOM | 6949 | N | TYR | 94 | 77.633 | 30.121 | 25.729 | 1.00 | 29.82 | X | N |
| ATOM | 6950 | CA | TYR | 94 | 77.210 | 31.143 | 24.774 | 1.00 | 29.82 | X | C |
| ATOM | 6951 | CB | TYR | 94 | 76.448 | 32.267 | 25.489 | 1.00 | 45.66 | X | C |
| ATOM | 6952 | CG | TYR | 94 | 75.282 | 31.829 | 26.343 | 1.00 | 45.66 | X | C |
| ATOM | 6953 | CD1 | TYR | 94 | 74.053 | 31.494 | 25.771 | 1.00 | 45.66 | X | C |
| ATOM | 6954 | CE1 | TYR | 94 | 72.979 | 31.108 | 26.564 | 1.00 | 45.66 | X | C |
| ATOM | 6955 | CD2 | TYR | 94 | 75.405 | 31.763 | 27.733 | 1.00 | 45.66 | X | C |
| ATOM | 6956 | CE2 | TYR | 94 | 74.342 | 31.376 | 28.532 | 1.00 | 45.66 | X | C |
| ATOM | 6957 | CZ | TYR | 94 | 73.132 | 31.051 | 27.943 | 1.00 | 45.66 | X | C |
| ATOM | 6958 | OH | TYR | 94 | 72.082 | 30.665 | 28.743 | 1.00 | 45.66 | X | O |
| ATOM | 6959 | C | TYR | 94 | 78.389 | 31.799 | 24.074 | 1.00 | 29.82 | X | C |
| ATOM | 6960 | O | TYR | 94 | 79.360 | 32.174 | 24.727 | 1.00 | 29.82 | X | O |
| ATOM | 6961 | N | CYS | 95 | 78.332 | 31.923 | 22.752 | 1.00 | 22.64 | X | N |
| ATOM | 6962 | CA | CYS | 95 | 79.394 | 32.659 | 22.091 | 1.00 | 22.64 | X | C |
| ATOM | 6963 | C | CYS | 95 | 78.871 | 34.094 | 22.103 | 1.00 | 22.64 | X | C |
| ATOM | 6964 | O | CYS | 95 | 77.656 | 34.337 | 22.170 | 1.00 | 22.64 | X | O |
| ATOM | 6965 | CB | CYS | 95 | 79.660 | 32.185 | 20.660 | 1.00 | 55.79 | X | C |
| ATOM | 6966 | SG | CYS | 95 | 78.222 | 31.748 | 19.650 | 1.00 | 55.79 | X | S |
| ATOM | 6967 | N | THR | 96 | 79.778 | 35.057 | 22.067 | 1.00 | 43.77 | X | N |
| ATOM | 6968 | CA | THR | 96 | 79.337 | 36.435 | 22.107 | 1.00 | 43.77 | X | C |
| ATOM | 6969 | CB | THR | 96 | 79.387 | 36.985 | 23.556 | 1.00 | 38.47 | X | C |
| ATOM | 6970 | OG1 | THR | 96 | 80.723 | 36.865 | 24.069 | 1.00 | 38.47 | X | O |
| ATOM | 6971 | CG2 | THR | 96 | 78.421 | 36.220 | 24.453 | 1.00 | 38.47 | X | C |
| ATOM | 6972 | C | THR | 96 | 80.130 | 37.370 | 21.220 | 1.00 | 43.77 | X | C |
| ATOM | 6973 | O | THR | 96 | 81.328 | 37.174 | 20.987 | 1.00 | 43.77 | X | O |
| ATOM | 6974 | N | ARG | 97 | 79.432 | 38.379 | 20.709 | 1.00 | 52.60 | X | N |
| ATOM | 6975 | CA | ARG | 97 | 80.068 | 39.400 | 19.899 | 1.00 | 52.60 | X | C |
| ATOM | 6976 | CB | ARG | 97 | 79.237 | 39.799 | 18.689 | 1.00 | 26.06 | X | C |
| ATOM | 6977 | CG | ARG | 97 | 80.052 | 40.645 | 17.733 | 1.00 | 26.06 | X | C |
| ATOM | 6978 | CD | ARG | 97 | 79.235 | 41.249 | 16.624 | 1.00 | 26.06 | X | C |
| ATOM | 6979 | NE | ARG | 97 | 78.494 | 42.412 | 17.074 | 1.00 | 26.06 | X | N |
| ATOM | 6980 | CZ | ARG | 97 | 77.853 | 43.231 | 16.255 | 1.00 | 26.06 | X | C |
| ATOM | 6981 | NH1 | ARG | 97 | 77.873 | 43.004 | 14.948 | 1.00 | 26.06 | X | N |
| ATOM | 6982 | NH2 | ARG | 97 | 77.187 | 44.271 | 16.742 | 1.00 | 26.06 | X | N |
| ATOM | 6983 | C | ARG | 97 | 80.142 | 40.590 | 20.820 | 1.00 | 52.60 | X | C |
| ATOM | 6984 | O | ARG | 97 | 79.116 | 41.100 | 21.260 | 1.00 | 52.60 | X | O |
| ATOM | 6985 | N | GLY | 98 | 81.353 | 41.020 | 21.129 | 1.00 | 31.82 | X | N |
| ATOM | 6986 | CA | GLY | 98 | 81.505 | 42.162 | 22.004 | 1.00 | 31.82 | X | C |
| ATOM | 6987 | C | GLY | 98 | 81.635 | 43.450 | 21.225 | 1.00 | 31.82 | X | C |
| ATOM | 6988 | O | GLY | 98 | 81.903 | 43.452 | 20.020 | 1.00 | 31.82 | X | O |
| ATOM | 6989 | N | PHE | 99 | 81.416 | 44.558 | 21.913 | 1.00 | 20.36 | X | N |
| ATOM | 6990 | CA | PHE | 99 | 81.554 | 45.859 | 21.289 | 1.00 | 20.36 | X | C |
| ATOM | 6991 | CB | PHE | 99 | 80.358 | 46.753 | 21.621 | 1.00 | 37.93 | X | C |
| ATOM | 6992 | CG | PHE | 99 | 80.633 | 48.214 | 21.431 | 1.00 | 37.93 | X | C |
| ATOM | 6993 | CD1 | PHE | 99 | 80.968 | 49.015 | 22.517 | 1.00 | 37.93 | X | C |
| ATOM | 6994 | CD2 | PHE | 99 | 80.606 | 48.783 | 20.158 | 1.00 | 37.93 | X | C |
| ATOM | 6995 | CE1 | PHE | 99 | 81.276 | 50.355 | 22.339 | 1.00 | 37.93 | X | C |
| ATOM | 6996 | CE2 | PHE | 99 | 80.913 | 50.127 | 19.967 | 1.00 | 37.93 | X | C |
| ATOM | 6997 | CZ | PHE | 99 | 81.250 | 50.914 | 21.058 | 1.00 | 37.93 | X | C |
| ATOM | 6998 | C | PHE | 99 | 82.836 | 46.468 | 21.835 | 1.00 | 20.36 | X | C |
| ATOM | 6999 | O | PHE | 99 | 83.239 | 46.164 | 22.969 | 1.00 | 20.36 | X | O |
| ATOM | 7000 | N | GLY | 100 | 83.480 | 47.309 | 21.030 | 1.00 | 25.28 | X | N |
| ATOM | 7001 | CA | GLY | 100 | 84.704 | 47.954 | 21.469 | 1.00 | 25.28 | X | C |
| ATOM | 7002 | C | GLY | 100 | 85.850 | 46.983 | 21.672 | 1.00 | 25.28 | X | C |
| ATOM | 7003 | O | GLY | 100 | 86.390 | 46.466 | 20.700 | 1.00 | 25.28 | X | O |
| ATOM | 7004 | N | ASP | 101 | 86.231 | 46.744 | 22.926 | 1.00 | 27.39 | X | N |
| ATOM | 7005 | CA | ASP | 101 | 87.315 | 45.814 | 23.233 | 1.00 | 27.39 | X | C |
| ATOM | 7006 | CB | ASP | 101 | 88.175 | 46.338 | 24.396 | 1.00 | 32.17 | X | C |
| ATOM | 7007 | CG | ASP | 101 | 89.037 | 47.540 | 24.013 | 1.00 | 32.17 | X | C |
| ATOM | 7008 | OD1 | ASP | 101 | 89.287 | 47.744 | 22.812 | 1.00 | 32.17 | X | O |

Fig. 19: A-97

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 7009 | OD2 | ASP | 101 | 89.483 | 48.274 | 24.920 | 1.00 | 32.17 | X | O |
| ATOM | 7010 | C | ASP | 101 | 86.773 | 44.418 | 23.596 | 1.00 | 27.39 | X | C |
| ATOM | 7011 | O | ASP | 101 | 87.549 | 43.518 | 23.929 | 1.00 | 27.39 | X | O |
| ATOM | 7012 | N | GLY | 102 | 85.449 | 44.250 | 23.538 | 1.00 | 18.22 | X | N |
| ATOM | 7013 | CA | GLY | 102 | 84.822 | 42.973 | 23.861 | 1.00 | 18.22 | X | C |
| ATOM | 7014 | C | GLY | 102 | 83.925 | 42.948 | 25.100 | 1.00 | 18.22 | X | C |
| ATOM | 7015 | O | GLY | 102 | 83.031 | 42.113 | 25.198 | 1.00 | 18.22 | X | O |
| ATOM | 7016 | N | GLY | 103 | 84.147 | 43.870 | 26.034 | 1.00 | 34.16 | X | N |
| ATOM | 7017 | CA | GLY | 103 | 83.370 | 43.915 | 27.268 | 1.00 | 34.16 | X | C |
| ATOM | 7018 | C | GLY | 103 | 81.850 | 43.964 | 27.216 | 1.00 | 34.16 | X | C |
| ATOM | 7019 | O | GLY | 103 | 81.182 | 43.416 | 28.087 | 1.00 | 34.16 | X | O |
| ATOM | 7020 | N | TYR | 104 | 81.290 | 44.649 | 26.230 | 1.00 | 25.31 | X | N |
| ATOM | 7021 | CA | TYR | 104 | 79.839 | 44.732 | 26.096 | 1.00 | 25.31 | X | C |
| ATOM | 7022 | CB | TYR | 104 | 79.433 | 46.131 | 25.639 | 1.00 | 26.21 | X | C |
| ATOM | 7023 | CG | TYR | 104 | 77.989 | 46.260 | 25.234 | 1.00 | 26.21 | X | C |
| ATOM | 7024 | CD1 | TYR | 104 | 77.635 | 46.980 | 24.087 | 1.00 | 26.21 | X | C |
| ATOM | 7025 | CE1 | TYR | 104 | 76.309 | 47.079 | 23.677 | 1.00 | 26.21 | X | C |
| ATOM | 7026 | CD2 | TYR | 104 | 76.972 | 45.646 | 25.972 | 1.00 | 26.21 | X | C |
| ATOM | 7027 | CE2 | TYR | 104 | 75.639 | 45.742 | 25.573 | 1.00 | 26.21 | X | C |
| ATOM | 7028 | CZ | TYR | 104 | 75.323 | 46.456 | 24.422 | 1.00 | 26.21 | X | C |
| ATOM | 7029 | OH | TYR | 104 | 74.025 | 46.523 | 23.995 | 1.00 | 26.21 | X | O |
| ATOM | 7030 | C | TYR | 104 | 79.484 | 43.700 | 25.037 | 1.00 | 25.31 | X | C |
| ATOM | 7031 | O | TYR | 104 | 79.905 | 43.810 | 23.886 | 1.00 | 25.31 | X | O |
| ATOM | 7032 | N | PHE | 105 | 78.728 | 42.686 | 25.432 | 1.00 | 17.54 | X | N |
| ATOM | 7033 | CA | PHE | 105 | 78.354 | 41.616 | 24.518 | 1.00 | 17.54 | X | C |
| ATOM | 7034 | CB | PHE | 105 | 78.088 | 40.337 | 25.309 | 1.00 | 20.12 | X | C |
| ATOM | 7035 | CG | PHE | 105 | 79.154 | 40.010 | 26.312 | 1.00 | 20.12 | X | C |
| ATOM | 7036 | CD1 | PHE | 105 | 80.478 | 39.817 | 25.908 | 1.00 | 20.12 | X | C |
| ATOM | 7037 | CD2 | PHE | 105 | 78.832 | 39.891 | 27.661 | 1.00 | 20.12 | X | C |
| ATOM | 7038 | CE1 | PHE | 105 | 81.472 | 39.511 | 26.836 | 1.00 | 20.12 | X | C |
| ATOM | 7039 | CE2 | PHE | 105 | 79.808 | 39.586 | 28.594 | 1.00 | 20.12 | X | C |
| ATOM | 7040 | CZ | PHE | 105 | 81.136 | 39.395 | 28.183 | 1.00 | 20.12 | X | C |
| ATOM | 7041 | C | PHE | 105 | 77.127 | 41.938 | 23.669 | 1.00 | 17.54 | X | C |
| ATOM | 7042 | O | PHE | 105 | 75.989 | 41.689 | 24.080 | 1.00 | 17.54 | X | O |
| ATOM | 7043 | N | ASP | 106 | 77.376 | 42.488 | 22.482 | 1.00 | 46.21 | X | N |
| ATOM | 7044 | CA | ASP | 106 | 76.327 | 42.840 | 21.532 | 1.00 | 46.21 | X | C |
| ATOM | 7045 | CB | ASP | 106 | 76.908 | 43.074 | 20.143 | 1.00 | 54.80 | X | C |
| ATOM | 7046 | CG | ASP | 106 | 77.456 | 44.442 | 19.976 | 1.00 | 54.80 | X | C |
| ATOM | 7047 | OD1 | ASP | 106 | 76.774 | 45.384 | 20.429 | 1.00 | 54.80 | X | O |
| ATOM | 7048 | OD2 | ASP | 106 | 78.552 | 44.576 | 19.387 | 1.00 | 54.80 | X | O |
| ATOM | 7049 | C | ASP | 106 | 75.355 | 41.705 | 21.399 | 1.00 | 46.21 | X | C |
| ATOM | 7050 | O | ASP | 106 | 74.281 | 41.707 | 21.974 | 1.00 | 46.21 | X | O |
| ATOM | 7051 | N | VAL | 107 | 75.769 | 40.732 | 20.603 | 1.00 | 33.04 | X | N |
| ATOM | 7052 | CA | VAL | 107 | 74.979 | 39.559 | 20.312 | 1.00 | 33.04 | X | C |
| ATOM | 7053 | CB | VAL | 107 | 75.180 | 39.152 | 18.858 | 1.00 | 31.62 | X | C |
| ATOM | 7054 | CG1 | VAL | 107 | 74.156 | 38.100 | 18.457 | 1.00 | 31.62 | X | C |
| ATOM | 7055 | CG2 | VAL | 107 | 75.092 | 40.388 | 17.980 | 1.00 | 31.62 | X | C |
| ATOM | 7056 | C | VAL | 107 | 75.322 | 38.379 | 21.197 | 1.00 | 33.04 | X | C |
| ATOM | 7057 | O | VAL | 107 | 76.413 | 38.296 | 21.763 | 1.00 | 33.04 | X | O |
| ATOM | 7058 | N | TRP | 108 | 74.359 | 37.474 | 21.306 | 1.00 | 37.95 | X | N |
| ATOM | 7059 | CA | TRP | 108 | 74.501 | 36.266 | 22.092 | 1.00 | 37.95 | X | C |
| ATOM | 7060 | CB | TRP | 108 | 73.674 | 36.351 | 23.372 | 1.00 | 32.89 | X | C |
| ATOM | 7061 | CG | TRP | 108 | 74.212 | 37.315 | 24.368 | 1.00 | 32.89 | X | C |
| ATOM | 7062 | CD2 | TRP | 108 | 74.712 | 37.004 | 25.668 | 1.00 | 32.89 | X | C |
| ATOM | 7063 | CE2 | TRP | 108 | 75.114 | 38.216 | 26.261 | 1.00 | 32.89 | X | C |
| ATOM | 7064 | CE3 | TRP | 108 | 74.861 | 35.816 | 26.390 | 1.00 | 32.89 | X | C |
| ATOM | 7065 | CD1 | TRP | 108 | 74.327 | 38.664 | 24.225 | 1.00 | 32.89 | X | C |
| ATOM | 7066 | NE1 | TRP | 108 | 74.867 | 39.216 | 25.358 | 1.00 | 32.89 | X | N |
| ATOM | 7067 | CZ2 | TRP | 108 | 75.655 | 38.278 | 27.543 | 1.00 | 32.89 | X | C |
| ATOM | 7068 | CZ3 | TRP | 108 | 75.402 | 35.878 | 27.670 | 1.00 | 32.89 | X | C |
| ATOM | 7069 | CH2 | TRP | 108 | 75.792 | 37.103 | 28.231 | 1.00 | 32.89 | X | C |
| ATOM | 7070 | C | TRP | 108 | 73.984 | 35.119 | 21.260 | 1.00 | 37.95 | X | C |
| ATOM | 7071 | O | TRP | 108 | 73.067 | 35.296 | 20.451 | 1.00 | 37.95 | X | O |
| ATOM | 7072 | N | GLY | 109 | 74.568 | 33.942 | 21.460 | 1.00 | 75.91 | X | N |
| ATOM | 7073 | CA | GLY | 109 | 74.124 | 32.770 | 20.732 | 1.00 | 75.91 | X | C |
| ATOM | 7074 | C | GLY | 109 | 72.791 | 32.307 | 21.288 | 1.00 | 75.91 | X | C |
| ATOM | 7075 | O | GLY | 109 | 71.997 | 33.114 | 21.780 | 1.00 | 75.91 | X | O |
| ATOM | 7076 | N | GLN | 110 | 72.537 | 31.007 | 21.207 | 1.00 | 35.37 | X | N |
| ATOM | 7077 | CA | GLN | 110 | 71.291 | 30.457 | 21.724 | 1.00 | 35.37 | X | C |
| ATOM | 7078 | CB | GLN | 110 | 70.652 | 29.498 | 20.714 | 1.00 | 98.79 | X | C |
| ATOM | 7079 | CG | GLN | 110 | 71.443 | 28.228 | 20.442 | 1.00 | 98.79 | X | C |
| ATOM | 7080 | CD | GLN | 110 | 72.597 | 28.441 | 19.485 | 1.00 | 98.79 | X | C |
| ATOM | 7081 | OE1 | GLN | 110 | 73.318 | 27.502 | 19.152 | 1.00 | 98.79 | X | O |

Fig. 19: A-98

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 7082 | NE2 | GLN | 110 | 72.775 | 29.675 | 19.031 | 1.00 | 98.79 | X | N |
| ATOM | 7083 | C | GLN | 110 | 71.610 | 29.708 | 23.004 | 1.00 | 35.37 | X | C |
| ATOM | 7084 | O | GLN | 110 | 70.793 | 29.626 | 23.918 | 1.00 | 35.37 | X | O |
| ATOM | 7085 | N | GLY | 111 | 72.831 | 29.194 | 23.067 | 1.00 | 45.85 | X | N |
| ATOM | 7086 | CA | GLY | 111 | 73.257 | 28.430 | 24.219 | 1.00 | 45.85 | X | C |
| ATOM | 7087 | C | GLY | 111 | 73.349 | 26.981 | 23.781 | 1.00 | 45.85 | X | C |
| ATOM | 7088 | O | GLY | 111 | 72.596 | 26.540 | 22.913 | 1.00 | 45.85 | X | O |
| ATOM | 7089 | N | THR | 112 | 74.281 | 26.243 | 24.369 | 1.00 | 30.06 | X | N |
| ATOM | 7090 | CA | THR | 112 | 74.480 | 24.840 | 24.040 | 1.00 | 30.06 | X | C |
| ATOM | 7091 | CB | THR | 112 | 75.550 | 24.696 | 22.962 | 1.00 | 24.67 | X | C |
| ATOM | 7092 | OG1 | THR | 112 | 75.636 | 23.327 | 22.562 | 1.00 | 24.67 | X | O |
| ATOM | 7093 | CG2 | THR | 112 | 76.903 | 25.177 | 23.487 | 1.00 | 24.67 | X | C |
| ATOM | 7094 | C | THR | 112 | 74.944 | 24.184 | 25.328 | 1.00 | 30.06 | X | C |
| ATOM | 7095 | O | THR | 112 | 75.883 | 24.658 | 25.960 | 1.00 | 30.06 | X | O |
| ATOM | 7096 | N | LEU | 113 | 74.292 | 23.102 | 25.725 | 1.00 | 42.99 | X | N |
| ATOM | 7097 | CA | LEU | 113 | 74.646 | 22.449 | 26.981 | 1.00 | 42.99 | X | C |
| ATOM | 7098 | CB | LEU | 113 | 73.434 | 21.652 | 27.499 | 1.00 | 32.90 | X | C |
| ATOM | 7099 | CG | LEU | 113 | 73.366 | 21.006 | 28.896 | 1.00 | 32.90 | X | C |
| ATOM | 7100 | CD1 | LEU | 113 | 73.914 | 19.580 | 28.860 | 1.00 | 32.90 | X | C |
| ATOM | 7101 | CD2 | LEU | 113 | 74.109 | 21.884 | 29.889 | 1.00 | 32.90 | X | C |
| ATOM | 7102 | C | LEU | 113 | 75.890 | 21.560 | 26.932 | 1.00 | 42.99 | X | C |
| ATOM | 7103 | O | LEU | 113 | 76.190 | 20.899 | 25.929 | 1.00 | 42.99 | X | O |
| ATOM | 7104 | N | VAL | 114 | 76.621 | 21.561 | 28.037 | 1.00 | 35.21 | X | N |
| ATOM | 7105 | CA | VAL | 114 | 77.815 | 20.754 | 28.141 | 1.00 | 35.21 | X | C |
| ATOM | 7106 | CB | VAL | 114 | 79.070 | 21.592 | 27.837 | 1.00 | 43.74 | X | C |
| ATOM | 7107 | CG1 | VAL | 114 | 80.324 | 20.909 | 28.384 | 1.00 | 43.74 | X | C |
| ATOM | 7108 | CG2 | VAL | 114 | 79.189 | 21.774 | 26.331 | 1.00 | 43.74 | X | C |
| ATOM | 7109 | C | VAL | 114 | 77.906 | 20.141 | 29.529 | 1.00 | 35.21 | X | C |
| ATOM | 7110 | O | VAL | 114 | 78.064 | 20.845 | 30.529 | 1.00 | 35.21 | X | O |
| ATOM | 7111 | N | THR | 115 | 77.788 | 18.819 | 29.575 | 1.00 | 58.81 | X | N |
| ATOM | 7112 | CA | THR | 115 | 77.855 | 18.099 | 30.829 | 1.00 | 58.81 | X | C |
| ATOM | 7113 | CB | THR | 115 | 76.717 | 17.098 | 30.956 | 1.00 | 63.66 | X | C |
| ATOM | 7114 | OG1 | THR | 115 | 75.549 | 17.620 | 30.311 | 1.00 | 63.66 | X | O |
| ATOM | 7115 | CG2 | THR | 115 | 76.412 | 16.849 | 32.422 | 1.00 | 63.66 | X | C |
| ATOM | 7116 | C | THR | 115 | 79.161 | 17.337 | 30.903 | 1.00 | 58.81 | X | C |
| ATOM | 7117 | O | THR | 115 | 79.831 | 17.121 | 29.893 | 1.00 | 58.81 | X | O |
| ATOM | 7118 | N | VAL | 116 | 79.516 | 16.933 | 32.114 | 1.00 | 73.79 | X | N |
| ATOM | 7119 | CA | VAL | 116 | 80.741 | 16.191 | 32.352 | 1.00 | 73.79 | X | C |
| ATOM | 7120 | CB | VAL | 116 | 81.899 | 17.135 | 32.747 | 1.00 | 46.90 | X | C |
| ATOM | 7121 | CG1 | VAL | 116 | 83.172 | 16.339 | 32.941 | 1.00 | 46.90 | X | C |
| ATOM | 7122 | CG2 | VAL | 116 | 82.101 | 18.194 | 31.667 | 1.00 | 46.90 | X | C |
| ATOM | 7123 | C | VAL | 116 | 80.478 | 15.202 | 33.482 | 1.00 | 73.79 | X | C |
| ATOM | 7124 | O | VAL | 116 | 80.382 | 15.584 | 34.649 | 1.00 | 73.79 | X | O |
| ATOM | 7125 | N | SER | 117 | 80.349 | 13.931 | 33.114 | 1.00 | 65.98 | X | N |
| ATOM | 7126 | CA | SER | 117 | 80.088 | 12.858 | 34.066 | 1.00 | 65.98 | X | C |
| ATOM | 7127 | CB | SER | 117 | 78.608 | 12.861 | 34.458 | 1.00 | 62.16 | X | C |
| ATOM | 7128 | OG | SER | 117 | 77.776 | 12.825 | 33.308 | 1.00 | 62.16 | X | O |
| ATOM | 7129 | C | SER | 117 | 80.454 | 11.521 | 33.427 | 1.00 | 65.98 | X | C |
| ATOM | 7130 | O | SER | 117 | 81.498 | 11.396 | 32.789 | 1.00 | 65.98 | X | O |
| ATOM | 7131 | N | SER | 118 | 79.587 | 10.524 | 33.594 | 1.00 | 80.64 | X | N |
| ATOM | 7132 | CA | SER | 118 | 79.828 | 9.208 | 33.014 | 1.00 | 80.64 | X | C |
| ATOM | 7133 | CB | SER | 118 | 80.556 | 8.329 | 34.031 | 1.00 | 66.12 | X | C |
| ATOM | 7134 | OG | SER | 118 | 81.771 | 8.944 | 34.438 | 1.00 | 66.12 | X | O |
| ATOM | 7135 | C | SER | 118 | 78.524 | 8.543 | 32.563 | 1.00 | 80.64 | X | C |
| ATOM | 7136 | O | SER | 118 | 77.445 | 9.021 | 32.973 | 1.00 | 79.69 | X | O |
| ATOM | 7137 | OXT | SER | 118 | 78.594 | 7.553 | 31.804 | 1.00 | 65.17 | X | O |
| ATOM | 7138 | CB | ILE | 2 | 85.629 | 44.767 | 39.417 | 1.00 | 24.34 | Y | C |
| ATOM | 7139 | CG2 | ILE | 2 | 84.329 | 45.456 | 39.830 | 1.00 | 24.34 | Y | C |
| ATOM | 7140 | CG1 | ILE | 2 | 86.754 | 45.793 | 39.275 | 1.00 | 24.34 | Y | C |
| ATOM | 7141 | CD1 | ILE | 2 | 86.473 | 46.861 | 38.237 | 1.00 | 24.34 | Y | C |
| ATOM | 7142 | C | ILE | 2 | 84.812 | 42.776 | 40.634 | 1.00 | 29.24 | Y | C |
| ATOM | 7143 | O | ILE | 2 | 84.508 | 41.962 | 39.756 | 1.00 | 29.24 | Y | O |
| ATOM | 7144 | N | ILE | 2 | 87.254 | 42.972 | 40.068 | 1.00 | 29.24 | Y | N |
| ATOM | 7145 | CA | ILE | 2 | 86.011 | 43.705 | 40.462 | 1.00 | 29.24 | Y | C |
| ATOM | 7146 | N | GLN | 3 | 84.122 | 42.926 | 41.761 | 1.00 | 42.94 | Y | N |
| ATOM | 7147 | CA | GLN | 3 | 82.960 | 42.107 | 42.070 | 1.00 | 42.94 | Y | C |
| ATOM | 7148 | CB | GLN | 3 | 83.156 | 41.435 | 43.434 | 1.00 | 85.86 | Y | C |
| ATOM | 7149 | CG | GLN | 3 | 82.045 | 40.492 | 43.850 | 1.00 | 85.86 | Y | C |
| ATOM | 7150 | CD | GLN | 3 | 82.371 | 39.747 | 45.131 | 1.00 | 85.86 | Y | C |
| ATOM | 7151 | OE1 | GLN | 3 | 81.534 | 39.028 | 45.670 | 1.00 | 85.86 | Y | O |
| ATOM | 7152 | NE2 | GLN | 3 | 83.597 | 39.911 | 45.621 | 1.00 | 85.86 | Y | N |
| ATOM | 7153 | C | GLN | 3 | 81.684 | 42.943 | 42.059 | 1.00 | 42.94 | Y | C |
| ATOM | 7154 | O | GLN | 3 | 81.626 | 44.026 | 42.645 | 1.00 | 42.94 | Y | O |

# Fig. 19: A-99

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 7155 | N | LEU | 4 | 80.666 | 42.426 | 41.380 | 1.00 | 33.35 | Y | N |
| ATOM | 7156 | CA | LEU | 4 | 79.378 | 43.098 | 41.269 | 1.00 | 33.35 | Y | C |
| ATOM | 7157 | CB | LEU | 4 | 78.954 | 43.160 | 39.800 | 1.00 | 47.12 | Y | C |
| ATOM | 7158 | CG | LEU | 4 | 79.344 | 44.389 | 38.979 | 1.00 | 47.12 | Y | C |
| ATOM | 7159 | CD1 | LEU | 4 | 80.683 | 44.945 | 39.443 | 1.00 | 47.12 | Y | C |
| ATOM | 7160 | CD2 | LEU | 4 | 79.370 | 44.008 | 37.512 | 1.00 | 47.12 | Y | C |
| ATOM | 7161 | C | LEU | 4 | 78.296 | 42.395 | 42.073 | 1.00 | 33.35 | Y | C |
| ATOM | 7162 | O | LEU | 4 | 78.012 | 41.215 | 41.852 | 1.00 | 33.35 | Y | O |
| ATOM | 7163 | N | THR | 5 | 77.691 | 43.129 | 43.001 | 1.00 | 42.53 | Y | N |
| ATOM | 7164 | CA | THR | 5 | 76.628 | 42.586 | 43.833 | 1.00 | 42.53 | Y | C |
| ATOM | 7165 | CB | THR | 5 | 77.100 | 42.482 | 45.315 | 1.00 | 37.95 | Y | C |
| ATOM | 7166 | OG1 | THR | 5 | 75.992 | 42.697 | 46.196 | 1.00 | 37.95 | Y | O |
| ATOM | 7167 | CG2 | THR | 5 | 78.209 | 43.479 | 45.604 | 1.00 | 37.95 | Y | C |
| ATOM | 7168 | C | THR | 5 | 75.348 | 43.426 | 43.699 | 1.00 | 42.53 | Y | C |
| ATOM | 7169 | O | THR | 5 | 75.306 | 44.593 | 44.089 | 1.00 | 42.53 | Y | O |
| ATOM | 7170 | N | GLN | 6 | 74.318 | 42.806 | 43.119 | 1.00 | 44.79 | Y | N |
| ATOM | 7171 | CA | GLN | 6 | 73.009 | 43.423 | 42.877 | 1.00 | 44.79 | Y | C |
| ATOM | 7172 | CB | GLN | 6 | 72.340 | 42.791 | 41.641 | 1.00 | 23.30 | Y | C |
| ATOM | 7173 | CG | GLN | 6 | 73.239 | 42.643 | 40.421 | 1.00 | 23.30 | Y | C |
| ATOM | 7174 | CD | GLN | 6 | 72.520 | 42.055 | 39.195 | 1.00 | 23.30 | Y | C |
| ATOM | 7175 | OE1 | GLN | 6 | 73.163 | 41.628 | 38.231 | 1.00 | 23.30 | Y | O |
| ATOM | 7176 | NE2 | GLN | 6 | 71.193 | 42.046 | 39.226 | 1.00 | 23.30 | Y | N |
| ATOM | 7177 | C | GLN | 6 | 72.050 | 43.274 | 44.061 | 1.00 | 44.79 | Y | C |
| ATOM | 7178 | O | GLN | 6 | 72.195 | 42.370 | 44.883 | 1.00 | 44.79 | Y | O |
| ATOM | 7179 | N | SER | 7 | 71.057 | 44.156 | 44.128 | 1.00 | 78.31 | Y | N |
| ATOM | 7180 | CA | SER | 7 | 70.069 | 44.113 | 45.201 | 1.00 | 78.31 | Y | C |
| ATOM | 7181 | CB | SER | 7 | 70.640 | 44.715 | 46.480 | 1.00 | 85.46 | Y | C |
| ATOM | 7182 | OG | SER | 7 | 71.028 | 46.058 | 46.262 | 1.00 | 85.46 | Y | O |
| ATOM | 7183 | C | SER | 7 | 68.797 | 44.855 | 44.824 | 1.00 | 78.31 | Y | C |
| ATOM | 7184 | O | SER | 7 | 68.847 | 45.923 | 44.220 | 1.00 | 78.31 | Y | O |
| ATOM | 7185 | N | PRO | 8 | 67.633 | 44.283 | 45.165 | 1.00 | 83.70 | Y | N |
| ATOM | 7186 | CD | PRO | 8 | 66.277 | 44.777 | 44.863 | 1.00 | 54.81 | Y | C |
| ATOM | 7187 | CA | PRO | 8 | 67.571 | 43.000 | 45.865 | 1.00 | 83.70 | Y | C |
| ATOM | 7188 | CB | PRO | 8 | 66.097 | 42.880 | 46.226 | 1.00 | 54.81 | Y | C |
| ATOM | 7189 | CG | PRO | 8 | 65.427 | 43.534 | 45.054 | 1.00 | 54.81 | Y | C |
| ATOM | 7190 | C | PRO | 8 | 68.015 | 41.895 | 44.925 | 1.00 | 83.70 | Y | C |
| ATOM | 7191 | O | PRO | 8 | 68.274 | 42.136 | 43.745 | 1.00 | 83.70 | Y | O |
| ATOM | 7192 | N | SER | 9 | 68.111 | 40.685 | 45.455 | 1.00 | 47.38 | Y | N |
| ATOM | 7193 | CA | SER | 9 | 68.504 | 39.541 | 44.651 | 1.00 | 47.38 | Y | C |
| ATOM | 7194 | CB | SER | 9 | 69.145 | 38.481 | 45.543 | 1.00 | 74.91 | Y | C |
| ATOM | 7195 | OG | SER | 9 | 70.214 | 39.045 | 46.283 | 1.00 | 74.91 | Y | O |
| ATOM | 7196 | C | SER | 9 | 67.232 | 39.002 | 44.025 | 1.00 | 47.38 | Y | C |
| ATOM | 7197 | O | SER | 9 | 67.237 | 38.434 | 42.936 | 1.00 | 47.38 | Y | O |
| ATOM | 7198 | N | SER | 10 | 66.134 | 39.214 | 44.736 | 1.00 | 60.45 | Y | N |
| ATOM | 7199 | CA | SER | 10 | 64.819 | 38.770 | 44.305 | 1.00 | 60.45 | Y | C |
| ATOM | 7200 | CB | SER | 10 | 64.476 | 37.449 | 44.991 | 1.00 | 51.82 | Y | C |
| ATOM | 7201 | OG | SER | 10 | 63.252 | 36.935 | 44.504 | 1.00 | 51.82 | Y | O |
| ATOM | 7202 | C | SER | 10 | 63.797 | 39.840 | 44.691 | 1.00 | 60.45 | Y | C |
| ATOM | 7203 | O | SER | 10 | 63.976 | 40.552 | 45.683 | 1.00 | 60.45 | Y | O |
| ATOM | 7204 | N | LEU | 11 | 62.730 | 39.964 | 43.910 | 1.00 | 65.48 | Y | N |
| ATOM | 7205 | CA | LEU | 11 | 61.710 | 40.964 | 44.206 | 1.00 | 65.48 | Y | C |
| ATOM | 7206 | CB | LEU | 11 | 62.206 | 42.366 | 43.830 | 1.00 | 51.28 | Y | C |
| ATOM | 7207 | CG | LEU | 11 | 62.310 | 42.727 | 42.342 | 1.00 | 51.28 | Y | C |
| ATOM | 7208 | CD1 | LEU | 11 | 60.949 | 43.139 | 41.803 | 1.00 | 51.28 | Y | C |
| ATOM | 7209 | CD2 | LEU | 11 | 63.294 | 43.877 | 42.168 | 1.00 | 51.28 | Y | C |
| ATOM | 7210 | C | LEU | 11 | 60.413 | 40.680 | 43.473 | 1.00 | 65.48 | Y | C |
| ATOM | 7211 | O | LEU | 11 | 60.412 | 40.363 | 42.282 | 1.00 | 65.48 | Y | O |
| ATOM | 7212 | N | SER | 12 | 59.305 | 40.803 | 44.189 | 1.00 | 84.56 | Y | N |
| ATOM | 7213 | CA | SER | 12 | 58.004 | 40.567 | 43.595 | 1.00 | 84.56 | Y | C |
| ATOM | 7214 | CB | SER | 12 | 57.209 | 39.578 | 44.445 | 1.00 | 71.89 | Y | C |
| ATOM | 7215 | OG | SER | 12 | 56.137 | 39.026 | 43.705 | 1.00 | 71.89 | Y | O |
| ATOM | 7216 | C | SER | 12 | 57.273 | 41.902 | 43.507 | 1.00 | 84.56 | Y | C |
| ATOM | 7217 | O | SER | 12 | 57.232 | 42.666 | 44.471 | 1.00 | 84.56 | Y | O |
| ATOM | 7218 | N | ALA | 13 | 56.713 | 42.192 | 42.341 | 1.00 | 109.71 | Y | N |
| ATOM | 7219 | CA | ALA | 13 | 55.997 | 43.442 | 42.152 | 1.00 | 109.71 | Y | C |
| ATOM | 7220 | CB | ALA | 13 | 56.947 | 44.509 | 41.632 | 1.00 | 88.46 | Y | C |
| ATOM | 7221 | C | ALA | 13 | 54.838 | 43.244 | 41.186 | 1.00 | 109.71 | Y | C |
| ATOM | 7222 | O | ALA | 13 | 54.869 | 42.347 | 40.341 | 1.00 | 109.71 | Y | O |
| ATOM | 7223 | N | SER | 14 | 53.816 | 44.084 | 41.315 | 1.00 | 66.55 | Y | N |
| ATOM | 7224 | CA | SER | 14 | 52.632 | 44.000 | 40.461 | 1.00 | 66.55 | Y | C |
| ATOM | 7225 | CB | SER | 14 | 51.370 | 44.265 | 41.290 | 1.00 | 62.23 | Y | C |
| ATOM | 7226 | OG | SER | 14 | 51.506 | 45.449 | 42.059 | 1.00 | 62.23 | Y | O |
| ATOM | 7227 | C | SER | 14 | 52.699 | 44.984 | 39.299 | 1.00 | 66.55 | Y | C |

# Fig. 19: A-100

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 7228 | O | SER | 14 | 53.362 | 46.015 | 39.394 | 1.00 | 66.55 | Y | O |
| ATOM | 7229 | N | VAL | 15 | 52.018 | 44.660 | 38.202 | 1.00 | 56.27 | Y | N |
| ATOM | 7230 | CA | VAL | 15 | 52.017 | 45.540 | 37.037 | 1.00 | 56.27 | Y | C |
| ATOM | 7231 | CB | VAL | 15 | 50.922 | 45.156 | 36.016 | 1.00 | 42.35 | Y | C |
| ATOM | 7232 | CG1 | VAL | 15 | 51.449 | 44.089 | 35.066 | 1.00 | 42.35 | Y | C |
| ATOM | 7233 | CG2 | VAL | 15 | 49.679 | 44.644 | 36.750 | 1.00 | 42.35 | Y | C |
| ATOM | 7234 | C | VAL | 15 | 51.773 | 46.964 | 37.492 | 1.00 | 56.27 | Y | C |
| ATOM | 7235 | O | VAL | 15 | 50.948 | 47.208 | 38.369 | 1.00 | 56.27 | Y | O |
| ATOM | 7236 | N | GLY | 16 | 52.509 | 47.903 | 36.911 | 1.00 | 54.44 | Y | N |
| ATOM | 7237 | CA | GLY | 16 | 52.343 | 49.296 | 37.280 | 1.00 | 54.44 | Y | C |
| ATOM | 7238 | C | GLY | 16 | 53.284 | 49.795 | 38.359 | 1.00 | 54.44 | Y | C |
| ATOM | 7239 | O | GLY | 16 | 53.419 | 51.000 | 38.542 | 1.00 | 54.44 | Y | O |
| ATOM | 7240 | N | ASP | 17 | 53.931 | 48.885 | 39.082 | 1.00 | 75.77 | Y | N |
| ATOM | 7241 | CA | ASP | 17 | 54.863 | 49.283 | 40.134 | 1.00 | 75.77 | Y | C |
| ATOM | 7242 | CB | ASP | 17 | 55.212 | 48.091 | 41.034 | 1.00 | 114.73 | Y | C |
| ATOM | 7243 | CG | ASP | 17 | 54.035 | 47.608 | 41.849 | 1.00 | 114.73 | Y | C |
| ATOM | 7244 | OD1 | ASP | 17 | 54.208 | 46.639 | 42.623 | 1.00 | 114.73 | Y | O |
| ATOM | 7245 | OD2 | ASP | 17 | 52.942 | 48.198 | 41.716 | 1.00 | 114.73 | Y | O |
| ATOM | 7246 | C | ASP | 17 | 56.149 | 49.824 | 39.525 | 1.00 | 75.77 | Y | C |
| ATOM | 7247 | O | ASP | 17 | 56.476 | 49.533 | 38.373 | 1.00 | 75.77 | Y | O |
| ATOM | 7248 | N | ARG | 18 | 56.873 | 50.616 | 40.304 | 1.00 | 69.15 | Y | N |
| ATOM | 7249 | CA | ARG | 18 | 58.139 | 51.161 | 39.844 | 1.00 | 69.15 | Y | C |
| ATOM | 7250 | CB | ARG | 18 | 58.263 | 52.634 | 40.225 | 1.00 | 52.23 | Y | C |
| ATOM | 7251 | CG | ARG | 18 | 59.557 | 53.291 | 39.779 | 1.00 | 52.23 | Y | C |
| ATOM | 7252 | CD | ARG | 18 | 59.365 | 54.788 | 39.625 | 1.00 | 52.23 | Y | C |
| ATOM | 7253 | NE | ARG | 18 | 60.622 | 55.478 | 39.370 | 1.00 | 52.23 | Y | N |
| ATOM | 7254 | CZ | ARG | 18 | 61.621 | 55.550 | 40.246 | 1.00 | 52.23 | Y | C |
| ATOM | 7255 | NH1 | ARG | 18 | 61.506 | 54.968 | 41.436 | 1.00 | 52.23 | Y | N |
| ATOM | 7256 | NH2 | ARG | 18 | 62.733 | 56.209 | 39.933 | 1.00 | 52.23 | Y | N |
| ATOM | 7257 | C | ARG | 18 | 59.232 | 50.346 | 40.514 | 1.00 | 69.15 | Y | C |
| ATOM | 7258 | O | ARG | 18 | 59.318 | 50.293 | 41.744 | 1.00 | 69.15 | Y | O |
| ATOM | 7259 | N | VAL | 19 | 60.064 | 49.706 | 39.701 | 1.00 | 58.62 | Y | N |
| ATOM | 7260 | CA | VAL | 19 | 61.132 | 48.871 | 40.221 | 1.00 | 58.62 | Y | C |
| ATOM | 7261 | CB | VAL | 19 | 61.068 | 47.477 | 39.567 | 1.00 | 74.00 | Y | C |
| ATOM | 7262 | CG1 | VAL | 19 | 62.050 | 46.531 | 40.235 | 1.00 | 74.00 | Y | C |
| ATOM | 7263 | CG2 | VAL | 19 | 59.651 | 46.938 | 39.664 | 1.00 | 74.00 | Y | C |
| ATOM | 7264 | C | VAL | 19 | 62.518 | 49.477 | 40.003 | 1.00 | 58.62 | Y | C |
| ATOM | 7265 | O | VAL | 19 | 62.782 | 50.096 | 38.975 | 1.00 | 58.62 | Y | O |
| ATOM | 7266 | N | THR | 20 | 63.399 | 49.297 | 40.978 | 1.00 | 54.75 | Y | N |
| ATOM | 7267 | CA | THR | 20 | 64.753 | 49.815 | 40.878 | 1.00 | 54.75 | Y | C |
| ATOM | 7268 | CB | THR | 20 | 64.883 | 51.148 | 41.639 | 1.00 | 56.43 | Y | C |
| ATOM | 7269 | OG1 | THR | 20 | 64.132 | 52.154 | 40.955 | 1.00 | 56.43 | Y | O |
| ATOM | 7270 | CG2 | THR | 20 | 66.337 | 51.586 | 41.726 | 1.00 | 56.43 | Y | C |
| ATOM | 7271 | C | THR | 20 | 65.806 | 48.834 | 41.401 | 1.00 | 54.75 | Y | C |
| ATOM | 7272 | O | THR | 20 | 65.963 | 48.663 | 42.611 | 1.00 | 54.75 | Y | O |
| ATOM | 7273 | N | ILE | 21 | 66.526 | 48.194 | 40.484 | 1.00 | 38.23 | Y | N |
| ATOM | 7274 | CA | ILE | 21 | 67.572 | 47.250 | 40.855 | 1.00 | 38.23 | Y | C |
| ATOM | 7275 | CB | ILE | 21 | 67.775 | 46.182 | 39.765 | 1.00 | 34.57 | Y | C |
| ATOM | 7276 | CG2 | ILE | 21 | 68.753 | 45.112 | 40.252 | 1.00 | 34.57 | Y | C |
| ATOM | 7277 | CG1 | ILE | 21 | 66.427 | 45.547 | 39.426 | 1.00 | 34.57 | Y | C |
| ATOM | 7278 | CD1 | ILE | 21 | 66.496 | 44.426 | 38.415 | 1.00 | 34.57 | Y | C |
| ATOM | 7279 | C | ILE | 21 | 68.877 | 48.006 | 41.047 | 1.00 | 38.23 | Y | C |
| ATOM | 7280 | O | ILE | 21 | 69.215 | 48.885 | 40.256 | 1.00 | 38.23 | Y | O |
| ATOM | 7281 | N | THR | 22 | 69.610 | 47.660 | 42.100 | 1.00 | 41.70 | Y | N |
| ATOM | 7282 | CA | THR | 22 | 70.880 | 48.312 | 42.396 | 1.00 | 41.70 | Y | C |
| ATOM | 7283 | CB | THR | 22 | 70.919 | 48.826 | 43.856 | 1.00 | 62.77 | Y | C |
| ATOM | 7284 | OG1 | THR | 22 | 69.986 | 49.903 | 44.017 | 1.00 | 62.77 | Y | O |
| ATOM | 7285 | CG2 | THR | 22 | 72.322 | 49.303 | 44.222 | 1.00 | 62.77 | Y | C |
| ATOM | 7286 | C | THR | 22 | 72.052 | 47.370 | 42.199 | 1.00 | 41.70 | Y | C |
| ATOM | 7287 | O | THR | 22 | 72.028 | 46.237 | 42.674 | 1.00 | 41.70 | Y | O |
| ATOM | 7288 | N | CYS | 23 | 73.077 | 47.852 | 41.500 | 1.00 | 52.46 | Y | N |
| ATOM | 7289 | CA | CYS | 23 | 74.289 | 47.076 | 41.247 | 1.00 | 52.46 | Y | C |
| ATOM | 7290 | C | CYS | 23 | 75.446 | 47.833 | 41.875 | 1.00 | 52.46 | Y | C |
| ATOM | 7291 | O | CYS | 23 | 75.749 | 48.957 | 41.476 | 1.00 | 52.46 | Y | O |
| ATOM | 7292 | CB | CYS | 23 | 74.522 | 46.938 | 39.744 | 1.00 | 61.15 | Y | C |
| ATOM | 7293 | SG | CYS | 23 | 75.983 | 45.982 | 39.184 | 1.00 | 61.15 | Y | S |
| ATOM | 7294 | N | SER | 24 | 76.079 | 47.219 | 42.866 | 1.00 | 43.95 | Y | N |
| ATOM | 7295 | CA | SER | 24 | 77.200 | 47.837 | 43.556 | 1.00 | 43.95 | Y | C |
| ATOM | 7296 | CB | SER | 24 | 76.992 | 47.751 | 45.072 | 1.00 | 58.07 | Y | C |
| ATOM | 7297 | OG | SER | 24 | 75.782 | 48.379 | 45.462 | 1.00 | 58.07 | Y | O |
| ATOM | 7298 | C | SER | 24 | 78.495 | 47.138 | 43.177 | 1.00 | 43.95 | Y | C |
| ATOM | 7299 | O | SER | 24 | 78.582 | 45.912 | 43.222 | 1.00 | 43.95 | Y | O |
| ATOM | 7300 | N | ALA | 25 | 79.503 | 47.924 | 42.814 | 1.00 | 35.63 | Y | N |

# Fig. 19: A-101

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 7301 | CA | ALA | 25 | 80.796 | 47.373 | 42.427 | 1.00 | 35.63 | Y | C |
| ATOM | 7302 | CB | ALA | 25 | 81.214 | 47.920 | 41.068 | 1.00 | 50.18 | Y | C |
| ATOM | 7303 | C | ALA | 25 | 81.894 | 47.635 | 43.454 | 1.00 | 35.63 | Y | C |
| ATOM | 7304 | O | ALA | 25 | 82.050 | 48.754 | 43.959 | 1.00 | 35.63 | Y | O |
| ATOM | 7305 | N | SER | 26 | 82.650 | 46.579 | 43.742 | 1.00 | 37.44 | Y | N |
| ATOM | 7306 | CA | SER | 26 | 83.746 | 46.616 | 44.697 | 1.00 | 37.44 | Y | C |
| ATOM | 7307 | CB | SER | 26 | 84.492 | 45.280 | 44.672 | 1.00 | 31.41 | Y | C |
| ATOM | 7308 | OG | SER | 26 | 85.018 | 45.005 | 43.381 | 1.00 | 31.41 | Y | O |
| ATOM | 7309 | C | SER | 26 | 84.718 | 47.745 | 44.393 | 1.00 | 37.44 | Y | C |
| ATOM | 7310 | O | SER | 26 | 85.358 | 48.286 | 45.297 | 1.00 | 37.44 | Y | O |
| ATOM | 7311 | N | SER | 27 | 84.835 | 48.088 | 43.116 | 1.00 | 70.39 | Y | N |
| ATOM | 7312 | CA | SER | 27 | 85.726 | 49.157 | 42.687 | 1.00 | 70.39 | Y | C |
| ATOM | 7313 | CB | SER | 27 | 86.941 | 48.581 | 41.954 | 1.00 | 53.81 | Y | C |
| ATOM | 7314 | OG | SER | 27 | 87.574 | 47.567 | 42.716 | 1.00 | 53.81 | Y | O |
| ATOM | 7315 | C | SER | 27 | 84.922 | 50.023 | 41.736 | 1.00 | 70.39 | Y | C |
| ATOM | 7316 | O | SER | 27 | 83.960 | 49.545 | 41.139 | 1.00 | 70.39 | Y | O |
| ATOM | 7317 | N | SER | 28 | 85.306 | 51.290 | 41.595 | 1.00 | 30.73 | Y | N |
| ATOM | 7318 | CA | SER | 28 | 84.598 | 52.194 | 40.695 | 1.00 | 30.73 | Y | C |
| ATOM | 7319 | CB | SER | 28 | 85.060 | 53.628 | 40.920 | 1.00 | 55.81 | Y | C |
| ATOM | 7320 | OG | SER | 28 | 86.448 | 53.723 | 40.688 | 1.00 | 55.81 | Y | O |
| ATOM | 7321 | C | SER | 28 | 84.824 | 51.813 | 39.230 | 1.00 | 30.73 | Y | C |
| ATOM | 7322 | O | SER | 28 | 85.873 | 51.287 | 38.863 | 1.00 | 30.73 | Y | O |
| ATOM | 7323 | N | VAL | 29 | 83.832 | 52.092 | 38.398 | 1.00 | 34.83 | Y | N |
| ATOM | 7324 | CA | VAL | 29 | 83.909 | 51.780 | 36.983 | 1.00 | 34.83 | Y | C |
| ATOM | 7325 | CB | VAL | 29 | 83.173 | 50.443 | 36.682 | 1.00 | 24.96 | Y | C |
| ATOM | 7326 | CG1 | VAL | 29 | 83.891 | 49.286 | 37.382 | 1.00 | 24.96 | Y | C |
| ATOM | 7327 | CG2 | VAL | 29 | 81.717 | 50.518 | 37.153 | 1.00 | 24.96 | Y | C |
| ATOM | 7328 | C | VAL | 29 | 83.267 | 52.929 | 36.208 | 1.00 | 34.83 | Y | C |
| ATOM | 7329 | O | VAL | 29 | 82.397 | 53.621 | 36.738 | 1.00 | 34.83 | Y | O |
| ATOM | 7330 | N | ASN | 30 | 83.689 | 53.134 | 34.963 | 1.00 | 19.83 | Y | N |
| ATOM | 7331 | CA | ASN | 30 | 83.152 | 54.225 | 34.145 | 1.00 | 19.83 | Y | C |
| ATOM | 7332 | CB | ASN | 30 | 84.086 | 54.517 | 32.963 | 1.00 | 44.92 | Y | C |
| ATOM | 7333 | CG | ASN | 30 | 84.524 | 53.261 | 32.254 | 1.00 | 44.92 | Y | C |
| ATOM | 7334 | OD1 | ASN | 30 | 85.235 | 52.431 | 32.832 | 1.00 | 44.92 | Y | O |
| ATOM | 7335 | ND2 | ASN | 30 | 84.097 | 53.099 | 31.001 | 1.00 | 44.92 | Y | N |
| ATOM | 7336 | C | ASN | 30 | 81.740 | 53.976 | 33.634 | 1.00 | 19.83 | Y | C |
| ATOM | 7337 | O | ASN | 30 | 80.998 | 54.926 | 33.381 | 1.00 | 19.83 | Y | O |
| ATOM | 7338 | N | HIS | 31 | 81.367 | 52.708 | 33.475 | 1.00 | 24.55 | Y | N |
| ATOM | 7339 | CA | HIS | 31 | 80.031 | 52.373 | 32.991 | 1.00 | 24.55 | Y | C |
| ATOM | 7340 | CB | HIS | 31 | 80.003 | 52.259 | 31.459 | 1.00 | 41.70 | Y | C |
| ATOM | 7341 | CG | HIS | 31 | 80.061 | 53.572 | 30.737 | 1.00 | 41.70 | Y | C |
| ATOM | 7342 | CD2 | HIS | 31 | 79.124 | 54.233 | 30.016 | 1.00 | 41.70 | Y | C |
| ATOM | 7343 | ND1 | HIS | 31 | 81.196 | 54.351 | 30.692 | 1.00 | 41.70 | Y | N |
| ATOM | 7344 | CE1 | HIS | 31 | 80.958 | 55.435 | 29.973 | 1.00 | 41.70 | Y | C |
| ATOM | 7345 | NE2 | HIS | 31 | 79.708 | 55.387 | 29.551 | 1.00 | 41.70 | Y | N |
| ATOM | 7346 | C | HIS | 31 | 79.548 | 51.058 | 33.567 | 1.00 | 24.55 | Y | C |
| ATOM | 7347 | O | HIS | 31 | 80.274 | 50.392 | 34.305 | 1.00 | 24.55 | Y | O |
| ATOM | 7348 | N | MET | 32 | 78.312 | 50.698 | 33.227 | 1.00 | 16.59 | Y | N |
| ATOM | 7349 | CA | MET | 32 | 77.719 | 49.440 | 33.664 | 1.00 | 16.59 | Y | C |
| ATOM | 7350 | CB | MET | 32 | 76.944 | 49.624 | 34.971 | 1.00 | 29.77 | Y | C |
| ATOM | 7351 | CG | MET | 32 | 76.606 | 48.310 | 35.684 | 1.00 | 29.77 | Y | C |
| ATOM | 7352 | SD | MET | 32 | 78.097 | 47.369 | 36.143 | 1.00 | 29.77 | Y | S |
| ATOM | 7353 | CE | MET | 32 | 78.855 | 48.463 | 37.337 | 1.00 | 29.77 | Y | C |
| ATOM | 7354 | C | MET | 32 | 76.779 | 48.941 | 32.563 | 1.00 | 16.59 | Y | C |
| ATOM | 7355 | O | MET | 32 | 76.138 | 49.734 | 31.871 | 1.00 | 16.59 | Y | O |
| ATOM | 7356 | N | PHE | 33 | 76.706 | 47.629 | 32.383 | 1.00 | 41.04 | Y | N |
| ATOM | 7357 | CA | PHE | 33 | 75.830 | 47.089 | 31.358 | 1.00 | 41.04 | Y | C |
| ATOM | 7358 | CB | PHE | 33 | 76.639 | 46.329 | 30.315 | 1.00 | 16.08 | Y | C |
| ATOM | 7359 | CG | PHE | 33 | 77.695 | 47.161 | 29.657 | 1.00 | 16.08 | Y | C |
| ATOM | 7360 | CD1 | PHE | 33 | 78.846 | 47.528 | 30.354 | 1.00 | 16.08 | Y | C |
| ATOM | 7361 | CD2 | PHE | 33 | 77.524 | 47.609 | 28.350 | 1.00 | 16.08 | Y | C |
| ATOM | 7362 | CE1 | PHE | 33 | 79.810 | 48.328 | 29.763 | 1.00 | 16.08 | Y | C |
| ATOM | 7363 | CE2 | PHE | 33 | 78.484 | 48.414 | 27.745 | 1.00 | 16.08 | Y | C |
| ATOM | 7364 | CZ | PHE | 33 | 79.634 | 48.776 | 28.456 | 1.00 | 16.08 | Y | C |
| ATOM | 7365 | C | PHE | 33 | 74.803 | 46.175 | 31.985 | 1.00 | 41.04 | Y | C |
| ATOM | 7366 | O | PHE | 33 | 75.036 | 45.622 | 33.057 | 1.00 | 41.04 | Y | O |
| ATOM | 7367 | N | TRP | 34 | 73.664 | 46.020 | 31.322 | 1.00 | 26.10 | Y | N |
| ATOM | 7368 | CA | TRP | 34 | 72.604 | 45.168 | 31.843 | 1.00 | 26.10 | Y | C |
| ATOM | 7369 | CB | TRP | 34 | 71.438 | 46.009 | 32.364 | 1.00 | 47.27 | Y | C |
| ATOM | 7370 | CG | TRP | 34 | 71.807 | 46.935 | 33.466 | 1.00 | 47.27 | Y | C |
| ATOM | 7371 | CD2 | TRP | 34 | 71.660 | 46.692 | 34.868 | 1.00 | 47.27 | Y | C |
| ATOM | 7372 | CE2 | TRP | 34 | 72.145 | 47.836 | 35.542 | 1.00 | 47.27 | Y | C |
| ATOM | 7373 | CE3 | TRP | 34 | 71.167 | 45.621 | 35.622 | 1.00 | 47.27 | Y | C |

# Fig. 19: A-102

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 7374 | CD1 | TRP | 34 | 72.360 | 48.175 | 33.346 | 1.00 | 47.27 | Y | C |
| ATOM | 7375 | NE1 | TRP | 34 | 72.567 | 48.725 | 34.589 | 1.00 | 47.27 | Y | N |
| ATOM | 7376 | CZ2 | TRP | 34 | 72.150 | 47.939 | 36.940 | 1.00 | 47.27 | Y | C |
| ATOM | 7377 | CZ3 | TRP | 34 | 71.172 | 45.725 | 37.013 | 1.00 | 47.27 | Y | C |
| ATOM | 7378 | CH2 | TRP | 34 | 71.661 | 46.879 | 37.655 | 1.00 | 47.27 | Y | C |
| ATOM | 7379 | C | TRP | 34 | 72.067 | 44.187 | 30.812 | 1.00 | 26.10 | Y | C |
| ATOM | 7380 | O | TRP | 34 | 71.904 | 44.513 | 29.630 | 1.00 | 26.10 | Y | O |
| ATOM | 7381 | N | TYR | 35 | 71.793 | 42.972 | 31.267 | 1.00 | 43.42 | Y | N |
| ATOM | 7382 | CA | TYR | 35 | 71.248 | 41.964 | 30.381 | 1.00 | 43.42 | Y | C |
| ATOM | 7383 | CB | TYR | 35 | 72.230 | 40.808 | 30.189 | 1.00 | 22.29 | Y | C |
| ATOM | 7384 | CG | TYR | 35 | 73.549 | 41.240 | 29.596 | 1.00 | 22.29 | Y | C |
| ATOM | 7385 | CD1 | TYR | 35 | 74.645 | 41.535 | 30.417 | 1.00 | 22.29 | Y | C |
| ATOM | 7386 | CE1 | TYR | 35 | 75.841 | 41.962 | 29.881 | 1.00 | 22.29 | Y | C |
| ATOM | 7387 | CD2 | TYR | 35 | 73.697 | 41.385 | 28.216 | 1.00 | 22.29 | Y | C |
| ATOM | 7388 | CE2 | TYR | 35 | 74.898 | 41.808 | 27.670 | 1.00 | 22.29 | Y | C |
| ATOM | 7389 | CZ | TYR | 35 | 75.960 | 42.094 | 28.510 | 1.00 | 22.29 | Y | C |
| ATOM | 7390 | OH | TYR | 35 | 77.148 | 42.516 | 27.972 | 1.00 | 22.29 | Y | O |
| ATOM | 7391 | C | TYR | 35 | 69.966 | 41.449 | 30.991 | 1.00 | 43.42 | Y | C |
| ATOM | 7392 | O | TYR | 35 | 69.826 | 41.393 | 32.214 | 1.00 | 43.42 | Y | O |
| ATOM | 7393 | N | GLN | 36 | 69.015 | 41.107 | 30.136 | 1.00 | 45.64 | Y | N |
| ATOM | 7394 | CA | GLN | 36 | 67.760 | 40.567 | 30.607 | 1.00 | 45.64 | Y | C |
| ATOM | 7395 | CB | GLN | 36 | 66.574 | 41.346 | 30.054 | 1.00 | 37.71 | Y | C |
| ATOM | 7396 | CG | GLN | 36 | 65.259 | 40.610 | 30.277 | 1.00 | 37.71 | Y | C |
| ATOM | 7397 | CD | GLN | 36 | 64.189 | 41.002 | 29.287 | 1.00 | 37.71 | Y | C |
| ATOM | 7398 | OE1 | GLN | 36 | 63.601 | 42.072 | 29.391 | 1.00 | 37.71 | Y | O |
| ATOM | 7399 | NE2 | GLN | 36 | 63.936 | 40.137 | 28.314 | 1.00 | 37.71 | Y | N |
| ATOM | 7400 | C | GLN | 36 | 67.664 | 39.138 | 30.118 | 1.00 | 45.64 | Y | C |
| ATOM | 7401 | O | GLN | 36 | 67.725 | 38.881 | 28.910 | 1.00 | 45.64 | Y | O |
| ATOM | 7402 | N | GLN | 37 | 67.522 | 38.205 | 31.050 | 1.00 | 50.28 | Y | N |
| ATOM | 7403 | CA | GLN | 37 | 67.390 | 36.809 | 30.670 | 1.00 | 50.28 | Y | C |
| ATOM | 7404 | CB | GLN | 37 | 68.522 | 35.961 | 31.265 | 1.00 | 34.85 | Y | C |
| ATOM | 7405 | CG | GLN | 37 | 68.392 | 34.487 | 30.904 | 1.00 | 34.85 | Y | C |
| ATOM | 7406 | CD | GLN | 37 | 69.543 | 33.645 | 31.388 | 1.00 | 34.85 | Y | C |
| ATOM | 7407 | OE1 | GLN | 37 | 69.925 | 33.699 | 32.565 | 1.00 | 34.85 | Y | O |
| ATOM | 7408 | NE2 | GLN | 37 | 70.098 | 32.842 | 30.484 | 1.00 | 34.85 | Y | N |
| ATOM | 7409 | C | GLN | 37 | 66.042 | 36.248 | 31.108 | 1.00 | 50.28 | Y | C |
| ATOM | 7410 | O | GLN | 37 | 65.690 | 36.272 | 32.293 | 1.00 | 50.28 | Y | O |
| ATOM | 7411 | N | LYS | 38 | 65.284 | 35.763 | 30.133 | 1.00 | 68.24 | Y | N |
| ATOM | 7412 | CA | LYS | 38 | 63.983 | 35.175 | 30.403 | 1.00 | 68.24 | Y | C |
| ATOM | 7413 | CB | LYS | 38 | 62.991 | 35.530 | 29.291 | 1.00 | 55.54 | Y | C |
| ATOM | 7414 | CG | LYS | 38 | 62.893 | 37.031 | 29.023 | 1.00 | 55.54 | Y | C |
| ATOM | 7415 | CD | LYS | 38 | 61.764 | 37.382 | 28.056 | 1.00 | 55.54 | Y | C |
| ATOM | 7416 | CE | LYS | 38 | 60.394 | 37.298 | 28.726 | 1.00 | 55.54 | Y | C |
| ATOM | 7417 | NZ | LYS | 38 | 60.290 | 38.166 | 29.943 | 1.00 | 55.54 | Y | N |
| ATOM | 7418 | C | LYS | 38 | 64.198 | 33.667 | 30.473 | 1.00 | 68.24 | Y | C |
| ATOM | 7419 | O | LYS | 38 | 64.971 | 33.104 | 29.696 | 1.00 | 68.24 | Y | O |
| ATOM | 7420 | N | PRO | 39 | 63.520 | 32.994 | 31.412 | 1.00 | 67.87 | Y | N |
| ATOM | 7421 | CD | PRO | 39 | 62.478 | 33.563 | 32.282 | 1.00 | 58.47 | Y | C |
| ATOM | 7422 | CA | PRO | 39 | 63.621 | 31.546 | 31.614 | 1.00 | 67.87 | Y | C |
| ATOM | 7423 | CB | PRO | 39 | 62.368 | 31.234 | 32.417 | 1.00 | 58.47 | Y | C |
| ATOM | 7424 | CG | PRO | 39 | 62.247 | 32.446 | 33.271 | 1.00 | 58.47 | Y | C |
| ATOM | 7425 | C | PRO | 39 | 63.717 | 30.714 | 30.338 | 1.00 | 67.87 | Y | C |
| ATOM | 7426 | O | PRO | 39 | 62.898 | 30.859 | 29.425 | 1.00 | 67.87 | Y | O |
| ATOM | 7427 | N | GLY | 40 | 64.730 | 29.847 | 30.288 | 1.00 | 54.98 | Y | N |
| ATOM | 7428 | CA | GLY | 40 | 64.925 | 28.977 | 29.137 | 1.00 | 54.98 | Y | C |
| ATOM | 7429 | C | GLY | 40 | 65.488 | 29.625 | 27.882 | 1.00 | 54.98 | Y | C |
| ATOM | 7430 | O | GLY | 40 | 65.625 | 28.957 | 26.855 | 1.00 | 54.98 | Y | O |
| ATOM | 7431 | N | LYS | 41 | 65.801 | 30.918 | 27.955 | 1.00 | 83.28 | Y | N |
| ATOM | 7432 | CA | LYS | 41 | 66.364 | 31.641 | 26.816 | 1.00 | 83.28 | Y | C |
| ATOM | 7433 | CB | LYS | 41 | 65.414 | 32.754 | 26.354 | 1.00 | 72.06 | Y | C |
| ATOM | 7434 | CG | LYS | 41 | 64.045 | 32.271 | 25.882 | 1.00 | 72.06 | Y | C |
| ATOM | 7435 | CD | LYS | 41 | 63.316 | 33.311 | 25.008 | 1.00 | 72.06 | Y | C |
| ATOM | 7436 | CE | LYS | 41 | 63.035 | 34.642 | 25.726 | 1.00 | 72.06 | Y | C |
| ATOM | 7437 | NZ | LYS | 41 | 64.229 | 35.536 | 25.855 | 1.00 | 72.06 | Y | N |
| ATOM | 7438 | C | LYS | 41 | 67.727 | 32.245 | 27.160 | 1.00 | 83.28 | Y | C |
| ATOM | 7439 | O | LYS | 41 | 68.110 | 32.327 | 28.331 | 1.00 | 83.28 | Y | O |
| ATOM | 7440 | N | ALA | 42 | 68.458 | 32.666 | 26.133 | 1.00 | 55.60 | Y | N |
| ATOM | 7441 | CA | ALA | 42 | 69.776 | 33.261 | 26.326 | 1.00 | 55.60 | Y | C |
| ATOM | 7442 | CB | ALA | 42 | 70.561 | 33.194 | 25.041 | 1.00 | 1.87 | Y | C |
| ATOM | 7443 | C | ALA | 42 | 69.623 | 34.707 | 26.754 | 1.00 | 55.60 | Y | C |
| ATOM | 7444 | O | ALA | 42 | 68.607 | 35.337 | 26.462 | 1.00 | 55.60 | Y | O |
| ATOM | 7445 | N | PRO | 43 | 70.628 | 35.259 | 27.455 | 1.00 | 54.21 | Y | N |
| ATOM | 7446 | CD | PRO | 43 | 71.849 | 34.627 | 27.983 | 1.00 | 18.24 | Y | C |

# Fig. 19: A-103

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 7447 | CA | PRO | 43 | 70.537 | 36.656 | 27.889 | 1.00 | 54.21 | Y | C |
| ATOM | 7448 | CB | PRO | 43 | 71.875 | 36.890 | 28.594 | 1.00 | 18.24 | Y | C |
| ATOM | 7449 | CG | PRO | 43 | 72.202 | 35.544 | 29.149 | 1.00 | 18.24 | Y | C |
| ATOM | 7450 | C | PRO | 43 | 70.349 | 37.584 | 26.689 | 1.00 | 54.21 | Y | C |
| ATOM | 7451 | O | PRO | 43 | 70.660 | 37.219 | 25.555 | 1.00 | 54.21 | Y | O |
| ATOM | 7452 | N | LYS | 44 | 69.837 | 38.782 | 26.946 | 1.00 | 55.44 | Y | N |
| ATOM | 7453 | CA | LYS | 44 | 69.618 | 39.764 | 25.892 | 1.00 | 55.44 | Y | C |
| ATOM | 7454 | CB | LYS | 44 | 68.120 | 39.894 | 25.601 | 1.00 | 46.11 | Y | C |
| ATOM | 7455 | CG | LYS | 44 | 67.705 | 39.473 | 24.199 | 1.00 | 46.11 | Y | C |
| ATOM | 7456 | CD | LYS | 44 | 66.189 | 39.520 | 24.018 | 1.00 | 46.11 | Y | C |
| ATOM | 7457 | CE | LYS | 44 | 65.457 | 38.464 | 24.865 | 1.00 | 46.11 | Y | C |
| ATOM | 7458 | NZ | LYS | 44 | 65.564 | 38.665 | 26.354 | 1.00 | 46.11 | Y | N |
| ATOM | 7459 | C | LYS | 44 | 70.172 | 41.117 | 26.328 | 1.00 | 55.44 | Y | C |
| ATOM | 7460 | O | LYS | 44 | 69.930 | 41.554 | 27.454 | 1.00 | 55.44 | Y | O |
| ATOM | 7461 | N | PRO | 45 | 70.946 | 41.785 | 25.451 | 1.00 | 21.39 | Y | N |
| ATOM | 7462 | CD | PRO | 45 | 71.303 | 41.365 | 24.085 | 1.00 | 11.37 | Y | C |
| ATOM | 7463 | CA | PRO | 45 | 71.523 | 43.103 | 25.772 | 1.00 | 21.39 | Y | C |
| ATOM | 7464 | CB | PRO | 45 | 72.159 | 43.539 | 24.457 | 1.00 | 11.37 | Y | C |
| ATOM | 7465 | CG | PRO | 45 | 72.485 | 42.234 | 23.795 | 1.00 | 11.37 | Y | C |
| ATOM | 7466 | C | PRO | 45 | 70.361 | 44.010 | 26.138 | 1.00 | 21.39 | Y | C |
| ATOM | 7467 | O | PRO | 45 | 69.407 | 44.103 | 25.383 | 1.00 | 21.39 | Y | O |
| ATOM | 7468 | N | TRP | 46 | 70.434 | 44.676 | 27.281 | 1.00 | 48.64 | Y | N |
| ATOM | 7469 | CA | TRP | 46 | 69.333 | 45.532 | 27.704 | 1.00 | 48.64 | Y | C |
| ATOM | 7470 | CB | TRP | 46 | 68.783 | 45.038 | 29.043 | 1.00 | 23.18 | Y | C |
| ATOM | 7471 | CG | TRP | 46 | 67.316 | 45.220 | 29.143 | 1.00 | 23.18 | Y | C |
| ATOM | 7472 | CD2 | TRP | 46 | 66.330 | 44.620 | 28.299 | 1.00 | 23.18 | Y | C |
| ATOM | 7473 | CE2 | TRP | 46 | 65.070 | 45.075 | 28.739 | 1.00 | 23.18 | Y | C |
| ATOM | 7474 | CE3 | TRP | 46 | 66.391 | 43.736 | 27.206 | 1.00 | 23.18 | Y | C |
| ATOM | 7475 | CD1 | TRP | 46 | 66.637 | 45.997 | 30.038 | 1.00 | 23.18 | Y | C |
| ATOM | 7476 | NE1 | TRP | 46 | 65.282 | 45.914 | 29.803 | 1.00 | 23.18 | Y | N |
| ATOM | 7477 | CZ2 | TRP | 46 | 63.881 | 44.679 | 28.126 | 1.00 | 23.18 | Y | C |
| ATOM | 7478 | CZ3 | TRP | 46 | 65.212 | 43.342 | 26.599 | 1.00 | 23.18 | Y | C |
| ATOM | 7479 | CH2 | TRP | 46 | 63.973 | 43.814 | 27.059 | 1.00 | 23.18 | Y | C |
| ATOM | 7480 | C | TRP | 46 | 69.694 | 47.007 | 27.826 | 1.00 | 48.64 | Y | C |
| ATOM | 7481 | O | TRP | 46 | 68.986 | 47.877 | 27.324 | 1.00 | 48.64 | Y | O |
| ATOM | 7482 | N | ILE | 47 | 70.785 | 47.283 | 28.523 | 1.00 | 42.06 | Y | N |
| ATOM | 7483 | CA | ILE | 47 | 71.238 | 48.644 | 28.717 | 1.00 | 42.06 | Y | C |
| ATOM | 7484 | CB | ILE | 47 | 70.801 | 49.172 | 30.099 | 1.00 | 37.03 | Y | C |
| ATOM | 7485 | CG2 | ILE | 47 | 71.345 | 50.580 | 30.325 | 1.00 | 37.03 | Y | C |
| ATOM | 7486 | CG1 | ILE | 47 | 69.275 | 49.168 | 30.198 | 1.00 | 37.03 | Y | C |
| ATOM | 7487 | CD1 | ILE | 47 | 68.749 | 49.670 | 31.538 | 1.00 | 37.03 | Y | C |
| ATOM | 7488 | C | ILE | 47 | 72.758 | 48.641 | 28.638 | 1.00 | 42.06 | Y | C |
| ATOM | 7489 | O | ILE | 47 | 73.417 | 47.951 | 29.414 | 1.00 | 42.06 | Y | O |
| ATOM | 7490 | N | TYR | 48 | 73.310 | 49.387 | 27.684 | 1.00 | 17.47 | Y | N |
| ATOM | 7491 | CA | TYR | 48 | 74.753 | 49.467 | 27.532 | 1.00 | 17.47 | Y | C |
| ATOM | 7492 | CB | TYR | 48 | 75.189 | 49.145 | 26.106 | 1.00 | 20.64 | Y | C |
| ATOM | 7493 | CG | TYR | 48 | 74.613 | 50.048 | 25.046 | 1.00 | 20.64 | Y | C |
| ATOM | 7494 | CD1 | TYR | 48 | 73.267 | 49.988 | 24.710 | 1.00 | 20.64 | Y | C |
| ATOM | 7495 | CE1 | TYR | 48 | 72.743 | 50.792 | 23.704 | 1.00 | 20.64 | Y | C |
| ATOM | 7496 | CD2 | TYR | 48 | 75.425 | 50.940 | 24.353 | 1.00 | 20.64 | Y | C |
| ATOM | 7497 | CE2 | TYR | 48 | 74.916 | 51.750 | 23.347 | 1.00 | 20.64 | Y | C |
| ATOM | 7498 | CZ | TYR | 48 | 73.573 | 51.671 | 23.028 | 1.00 | 20.64 | Y | C |
| ATOM | 7499 | OH | TYR | 48 | 73.051 | 52.476 | 22.045 | 1.00 | 20.64 | Y | O |
| ATOM | 7500 | C | TYR | 48 | 75.193 | 50.861 | 27.892 | 1.00 | 17.47 | Y | C |
| ATOM | 7501 | O | TYR | 48 | 74.365 | 51.754 | 28.021 | 1.00 | 17.47 | Y | O |
| ATOM | 7502 | N | LEU | 49 | 76.497 | 51.044 | 28.054 | 1.00 | 31.07 | Y | N |
| ATOM | 7503 | CA | LEU | 49 | 77.042 | 52.337 | 28.429 | 1.00 | 31.07 | Y | C |
| ATOM | 7504 | CB | LEU | 49 | 77.200 | 53.247 | 27.205 | 1.00 | 20.44 | Y | C |
| ATOM | 7505 | CG | LEU | 49 | 78.368 | 53.044 | 26.236 | 1.00 | 20.44 | Y | C |
| ATOM | 7506 | CD1 | LEU | 49 | 79.662 | 52.870 | 27.019 | 1.00 | 20.44 | Y | C |
| ATOM | 7507 | CD2 | LEU | 49 | 78.121 | 51.836 | 25.385 | 1.00 | 20.44 | Y | C |
| ATOM | 7508 | C | LEU | 49 | 76.173 | 53.037 | 29.475 | 1.00 | 31.07 | Y | C |
| ATOM | 7509 | O | LEU | 49 | 75.769 | 54.178 | 29.293 | 1.00 | 31.07 | Y | O |
| ATOM | 7510 | N | THR | 50 | 75.861 | 52.329 | 30.555 | 1.00 | 28.24 | Y | N |
| ATOM | 7511 | CA | THR | 50 | 75.083 | 52.870 | 31.670 | 1.00 | 28.24 | Y | C |
| ATOM | 7512 | CB | THR | 50 | 75.754 | 54.128 | 32.230 | 1.00 | 41.62 | Y | C |
| ATOM | 7513 | OG1 | THR | 50 | 77.134 | 53.847 | 32.495 | 1.00 | 41.62 | Y | O |
| ATOM | 7514 | CG2 | THR | 50 | 75.066 | 54.568 | 33.522 | 1.00 | 41.62 | Y | C |
| ATOM | 7515 | C | THR | 50 | 73.605 | 53.187 | 31.485 | 1.00 | 28.24 | Y | C |
| ATOM | 7516 | O | THR | 50 | 72.761 | 52.603 | 32.158 | 1.00 | 28.24 | Y | O |
| ATOM | 7517 | N | SER | 51 | 73.283 | 54.114 | 30.595 | 1.00 | 28.33 | Y | N |
| ATOM | 7518 | CA | SER | 51 | 71.889 | 54.496 | 30.402 | 1.00 | 28.33 | Y | C |
| ATOM | 7519 | CB | SER | 51 | 71.729 | 55.981 | 30.714 | 1.00 | 81.44 | Y | C |

Fig. 19: A-104

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 7520 | OG | SER | 51 | 72.714 | 56.738 | 30.034 | 1.00 | 81.44 | Y | O |
| ATOM | 7521 | C | SER | 51 | 71.312 | 54.190 | 29.019 | 1.00 | 28.33 | Y | C |
| ATOM | 7522 | O | SER | 51 | 70.092 | 54.174 | 28.831 | 1.00 | 28.33 | Y | O |
| ATOM | 7523 | N | ASN | 52 | 72.184 | 53.941 | 28.053 | 1.00 | 27.44 | Y | N |
| ATOM | 7524 | CA | ASN | 52 | 71.736 | 53.648 | 26.704 | 1.00 | 27.44 | Y | C |
| ATOM | 7525 | CB | ASN | 52 | 72.942 | 53.523 | 25.779 | 1.00 | 42.81 | Y | C |
| ATOM | 7526 | CG | ASN | 52 | 73.623 | 54.849 | 25.546 | 1.00 | 42.81 | Y | C |
| ATOM | 7527 | OD1 | ASN | 52 | 73.059 | 55.733 | 24.907 | 1.00 | 42.81 | Y | O |
| ATOM | 7528 | ND2 | ASN | 52 | 74.829 | 55.006 | 26.076 | 1.00 | 42.81 | Y | N |
| ATOM | 7529 | C | ASN | 52 | 70.896 | 52.390 | 26.623 | 1.00 | 27.44 | Y | C |
| ATOM | 7530 | O | ASN | 52 | 71.336 | 51.320 | 27.027 | 1.00 | 27.44 | Y | O |
| ATOM | 7531 | N | LEU | 53 | 69.682 | 52.519 | 26.100 | 1.00 | 46.42 | Y | N |
| ATOM | 7532 | CA | LEU | 53 | 68.805 | 51.367 | 25.954 | 1.00 | 46.42 | Y | C |
| ATOM | 7533 | CB | LEU | 53 | 67.349 | 51.803 | 25.887 | 1.00 | 19.90 | Y | C |
| ATOM | 7534 | CG | LEU | 53 | 66.763 | 52.595 | 27.051 | 1.00 | 19.90 | Y | C |
| ATOM | 7535 | CD1 | LEU | 53 | 65.255 | 52.685 | 26.846 | 1.00 | 19.90 | Y | C |
| ATOM | 7536 | CD2 | LEU | 53 | 67.071 | 51.918 | 28.382 | 1.00 | 19.90 | Y | C |
| ATOM | 7537 | C | LEU | 53 | 69.136 | 50.610 | 24.676 | 1.00 | 46.42 | Y | C |
| ATOM | 7538 | O | LEU | 53 | 69.414 | 51.220 | 23.644 | 1.00 | 46.42 | Y | O |
| ATOM | 7539 | N | ALA | 54 | 69.101 | 49.281 | 24.744 | 1.00 | 35.05 | Y | N |
| ATOM | 7540 | CA | ALA | 54 | 69.378 | 48.447 | 23.583 | 1.00 | 35.05 | Y | C |
| ATOM | 7541 | CB | ALA | 54 | 69.220 | 46.994 | 23.930 | 1.00 | 27.54 | Y | C |
| ATOM | 7542 | C | ALA | 54 | 68.373 | 48.829 | 22.530 | 1.00 | 35.05 | Y | C |
| ATOM | 7543 | O | ALA | 54 | 67.680 | 49.834 | 22.666 | 1.00 | 35.05 | Y | O |
| ATOM | 7544 | N | SER | 55 | 68.259 | 48.026 | 21.486 | 1.00 | 47.40 | Y | N |
| ATOM | 7545 | CA | SER | 55 | 67.319 | 48.376 | 20.443 | 1.00 | 47.40 | Y | C |
| ATOM | 7546 | CB | SER | 55 | 67.689 | 47.681 | 19.140 | 1.00 | 36.06 | Y | C |
| ATOM | 7547 | OG | SER | 55 | 67.083 | 48.359 | 18.051 | 1.00 | 36.06 | Y | O |
| ATOM | 7548 | C | SER | 55 | 65.866 | 48.073 | 20.801 | 1.00 | 47.40 | Y | C |
| ATOM | 7549 | O | SER | 55 | 64.993 | 48.921 | 20.631 | 1.00 | 47.40 | Y | O |
| ATOM | 7550 | N | GLY | 56 | 65.599 | 46.878 | 21.312 | 1.00 | 54.09 | Y | N |
| ATOM | 7551 | CA | GLY | 56 | 64.225 | 46.531 | 21.647 | 1.00 | 54.09 | Y | C |
| ATOM | 7552 | C | GLY | 56 | 63.650 | 47.071 | 22.948 | 1.00 | 54.09 | Y | C |
| ATOM | 7553 | O | GLY | 56 | 62.457 | 47.370 | 23.025 | 1.00 | 54.09 | Y | O |
| ATOM | 7554 | N | VAL | 57 | 64.497 | 47.197 | 23.965 | 1.00 | 63.10 | Y | N |
| ATOM | 7555 | CA | VAL | 57 | 64.082 | 47.667 | 25.282 | 1.00 | 63.10 | Y | C |
| ATOM | 7556 | CB | VAL | 57 | 65.311 | 48.113 | 26.120 | 1.00 | 46.15 | Y | C |
| ATOM | 7557 | CG1 | VAL | 57 | 64.923 | 48.248 | 27.588 | 1.00 | 46.15 | Y | C |
| ATOM | 7558 | CG2 | VAL | 57 | 66.446 | 47.118 | 25.961 | 1.00 | 46.15 | Y | C |
| ATOM | 7559 | C | VAL | 57 | 63.071 | 48.817 | 25.251 | 1.00 | 63.10 | Y | C |
| ATOM | 7560 | O | VAL | 57 | 63.363 | 49.898 | 24.747 | 1.00 | 63.10 | Y | O |
| ATOM | 7561 | N | PRO | 58 | 61.862 | 48.594 | 25.791 | 1.00 | 51.01 | Y | N |
| ATOM | 7562 | CD | PRO | 58 | 61.362 | 47.365 | 26.426 | 1.00 | 31.12 | Y | C |
| ATOM | 7563 | CA | PRO | 58 | 60.834 | 49.639 | 25.815 | 1.00 | 51.01 | Y | C |
| ATOM | 7564 | CB | PRO | 58 | 59.634 | 48.929 | 26.433 | 1.00 | 31.12 | Y | C |
| ATOM | 7565 | CG | PRO | 58 | 60.258 | 47.899 | 27.300 | 1.00 | 31.12 | Y | C |
| ATOM | 7566 | C | PRO | 58 | 61.305 | 50.829 | 26.643 | 1.00 | 51.01 | Y | C |
| ATOM | 7567 | O | PRO | 58 | 61.992 | 50.660 | 27.653 | 1.00 | 51.01 | Y | O |
| ATOM | 7568 | N | SER | 59 | 60.918 | 52.027 | 26.216 | 1.00 | 33.61 | Y | N |
| ATOM | 7569 | CA | SER | 59 | 61.330 | 53.267 | 26.874 | 1.00 | 33.61 | Y | C |
| ATOM | 7570 | CB | SER | 59 | 60.780 | 54.482 | 26.113 | 1.00 | 61.12 | Y | C |
| ATOM | 7571 | OG | SER | 59 | 59.368 | 54.481 | 26.096 | 1.00 | 61.12 | Y | O |
| ATOM | 7572 | C | SER | 59 | 61.023 | 53.411 | 28.359 | 1.00 | 33.61 | Y | C |
| ATOM | 7573 | O | SER | 59 | 61.495 | 54.353 | 28.990 | 1.00 | 33.61 | Y | O |
| ATOM | 7574 | N | ARG | 60 | 60.244 | 52.500 | 28.928 | 1.00 | 39.70 | Y | N |
| ATOM | 7575 | CA | ARG | 60 | 59.963 | 52.599 | 30.359 | 1.00 | 39.70 | Y | C |
| ATOM | 7576 | CB | ARG | 60 | 58.764 | 51.731 | 30.751 | 1.00 | 42.51 | Y | C |
| ATOM | 7577 | CG | ARG | 60 | 58.846 | 50.293 | 30.287 | 1.00 | 42.51 | Y | C |
| ATOM | 7578 | CD | ARG | 60 | 57.798 | 49.425 | 30.971 | 1.00 | 42.51 | Y | C |
| ATOM | 7579 | NE | ARG | 60 | 57.683 | 48.120 | 30.333 | 1.00 | 42.51 | Y | N |
| ATOM | 7580 | CZ | ARG | 60 | 57.277 | 47.939 | 29.079 | 1.00 | 42.51 | Y | C |
| ATOM | 7581 | NH1 | ARG | 60 | 56.943 | 48.979 | 28.324 | 1.00 | 42.51 | Y | N |
| ATOM | 7582 | NH2 | ARG | 60 | 57.210 | 46.718 | 28.569 | 1.00 | 42.51 | Y | N |
| ATOM | 7583 | C | ARG | 60 | 61.202 | 52.180 | 31.158 | 1.00 | 39.70 | Y | C |
| ATOM | 7584 | O | ARG | 60 | 61.311 | 52.451 | 32.357 | 1.00 | 39.70 | Y | O |
| ATOM | 7585 | N | PHE | 61 | 62.136 | 51.522 | 30.480 | 1.00 | 40.60 | Y | N |
| ATOM | 7586 | CA | PHE | 61 | 63.372 | 51.086 | 31.109 | 1.00 | 40.60 | Y | C |
| ATOM | 7587 | CB | PHE | 61 | 63.965 | 49.886 | 30.370 | 1.00 | 38.42 | Y | C |
| ATOM | 7588 | CG | PHE | 61 | 63.416 | 48.563 | 30.811 | 1.00 | 38.42 | Y | C |
| ATOM | 7589 | CD1 | PHE | 61 | 62.493 | 47.881 | 30.028 | 1.00 | 38.42 | Y | C |
| ATOM | 7590 | CD2 | PHE | 61 | 63.830 | 47.997 | 32.010 | 1.00 | 38.42 | Y | C |
| ATOM | 7591 | CE1 | PHE | 61 | 61.990 | 46.652 | 30.434 | 1.00 | 38.42 | Y | C |
| ATOM | 7592 | CE2 | PHE | 61 | 63.332 | 46.770 | 32.423 | 1.00 | 38.42 | Y | C |

# Fig. 19: A-105

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 7593 | CZ | PHE | 61 | 62.410 | 46.096 | 31.634 | 1.00 | 38.42 | Y | C |
| ATOM | 7594 | C | PHE | 61 | 64.399 | 52.209 | 31.097 | 1.00 | 40.60 | Y | C |
| ATOM | 7595 | O | PHE | 61 | 64.470 | 52.989 | 30.144 | 1.00 | 40.60 | Y | O |
| ATOM | 7596 | N | SER | 62 | 65.202 | 52.284 | 32.152 | 1.00 | 26.58 | Y | N |
| ATOM | 7597 | CA | SER | 62 | 66.238 | 53.306 | 32.247 | 1.00 | 26.58 | Y | C |
| ATOM | 7598 | CB | SER | 62 | 65.658 | 54.604 | 32.802 | 1.00 | 47.08 | Y | C |
| ATOM | 7599 | OG | SER | 62 | 65.071 | 54.395 | 34.076 | 1.00 | 47.08 | Y | O |
| ATOM | 7600 | C | SER | 62 | 67.376 | 52.828 | 33.145 | 1.00 | 26.58 | Y | C |
| ATOM | 7601 | O | SER | 62 | 67.160 | 52.123 | 34.125 | 1.00 | 26.58 | Y | O |
| ATOM | 7602 | N | GLY | 63 | 68.595 | 53.208 | 32.797 | 1.00 | 30.78 | Y | N |
| ATOM | 7603 | CA | GLY | 63 | 69.738 | 52.810 | 33.591 | 1.00 | 30.78 | Y | C |
| ATOM | 7604 | C | GLY | 63 | 70.426 | 54.067 | 34.056 | 1.00 | 30.78 | Y | C |
| ATOM | 7605 | O | GLY | 63 | 70.266 | 55.122 | 33.442 | 1.00 | 30.78 | Y | O |
| ATOM | 7606 | N | SER | 64 | 71.195 | 53.964 | 35.130 | 1.00 | 54.48 | Y | N |
| ATOM | 7607 | CA | SER | 64 | 71.884 | 55.130 | 35.652 | 1.00 | 54.48 | Y | C |
| ATOM | 7608 | CB | SER | 64 | 70.869 | 56.075 | 36.290 | 1.00 | 25.06 | Y | C |
| ATOM | 7609 | OG | SER | 64 | 71.519 | 57.204 | 36.839 | 1.00 | 25.06 | Y | O |
| ATOM | 7610 | C | SER | 64 | 72.947 | 54.763 | 36.675 | 1.00 | 54.48 | Y | C |
| ATOM | 7611 | O | SER | 64 | 73.000 | 53.632 | 37.154 | 1.00 | 54.48 | Y | O |
| ATOM | 7612 | N | GLY | 65 | 73.793 | 55.732 | 37.007 | 1.00 | 43.76 | Y | N |
| ATOM | 7613 | CA | GLY | 65 | 74.836 | 55.494 | 37.984 | 1.00 | 43.76 | Y | C |
| ATOM | 7614 | C | GLY | 65 | 76.218 | 56.023 | 37.637 | 1.00 | 43.76 | Y | C |
| ATOM | 7615 | O | GLY | 65 | 76.431 | 56.698 | 36.622 | 1.00 | 43.76 | Y | O |
| ATOM | 7616 | N | SER | 66 | 77.167 | 55.703 | 38.508 | 1.00 | 27.01 | Y | N |
| ATOM | 7617 | CA | SER | 66 | 78.546 | 56.110 | 38.339 | 1.00 | 27.01 | Y | C |
| ATOM | 7618 | CB | SER | 66 | 78.641 | 57.635 | 38.286 | 1.00 | 58.01 | Y | C |
| ATOM | 7619 | OG | SER | 66 | 77.927 | 58.229 | 39.355 | 1.00 | 58.01 | Y | O |
| ATOM | 7620 | C | SER | 66 | 79.367 | 55.563 | 39.498 | 1.00 | 27.01 | Y | C |
| ATOM | 7621 | O | SER | 66 | 78.817 | 55.039 | 40.464 | 1.00 | 27.01 | Y | O |
| ATOM | 7622 | N | GLY | 67 | 80.685 | 55.668 | 39.385 | 1.00 | 73.15 | Y | N |
| ATOM | 7623 | CA | GLY | 67 | 81.555 | 55.179 | 40.436 | 1.00 | 73.15 | Y | C |
| ATOM | 7624 | C | GLY | 67 | 81.312 | 53.733 | 40.822 | 1.00 | 73.15 | Y | C |
| ATOM | 7625 | O | GLY | 67 | 81.609 | 52.814 | 40.056 | 1.00 | 73.15 | Y | O |
| ATOM | 7626 | N | THR | 68 | 80.758 | 53.530 | 42.011 | 1.00 | 44.05 | Y | N |
| ATOM | 7627 | CA | THR | 68 | 80.506 | 52.186 | 42.506 | 1.00 | 44.05 | Y | C |
| ATOM | 7628 | CB | THR | 68 | 81.118 | 52.003 | 43.894 | 1.00 | 42.61 | Y | C |
| ATOM | 7629 | OG1 | THR | 68 | 80.524 | 52.945 | 44.793 | 1.00 | 42.61 | Y | O |
| ATOM | 7630 | CG2 | THR | 68 | 82.627 | 52.225 | 43.845 | 1.00 | 42.61 | Y | C |
| ATOM | 7631 | C | THR | 68 | 79.042 | 51.786 | 42.592 | 1.00 | 44.05 | Y | C |
| ATOM | 7632 | O | THR | 68 | 78.743 | 50.632 | 42.879 | 1.00 | 44.05 | Y | O |
| ATOM | 7633 | N | ASP | 69 | 78.128 | 52.720 | 42.352 | 1.00 | 35.15 | Y | N |
| ATOM | 7634 | CA | ASP | 69 | 76.708 | 52.392 | 42.424 | 1.00 | 35.15 | Y | C |
| ATOM | 7635 | CB | ASP | 69 | 76.066 | 53.103 | 43.617 | 1.00 | 108.02 | Y | C |
| ATOM | 7636 | CG | ASP | 69 | 76.592 | 52.591 | 44.946 | 1.00 | 108.02 | Y | C |
| ATOM | 7637 | OD1 | ASP | 69 | 76.357 | 51.406 | 45.268 | 1.00 | 108.02 | Y | O |
| ATOM | 7638 | OD2 | ASP | 69 | 77.249 | 53.370 | 45.667 | 1.00 | 108.02 | Y | O |
| ATOM | 7639 | C | ASP | 69 | 75.942 | 52.705 | 41.139 | 1.00 | 35.15 | Y | C |
| ATOM | 7640 | O | ASP | 69 | 75.884 | 53.850 | 40.693 | 1.00 | 35.15 | Y | O |
| ATOM | 7641 | N | TYR | 70 | 75.359 | 51.664 | 40.551 | 1.00 | 27.55 | Y | N |
| ATOM | 7642 | CA | TYR | 70 | 74.599 | 51.787 | 39.317 | 1.00 | 27.55 | Y | C |
| ATOM | 7643 | CB | TYR | 70 | 75.315 | 51.016 | 38.191 | 1.00 | 25.09 | Y | C |
| ATOM | 7644 | CG | TYR | 70 | 76.543 | 51.737 | 37.662 | 1.00 | 25.09 | Y | C |
| ATOM | 7645 | CD1 | TYR | 70 | 76.447 | 52.637 | 36.596 | 1.00 | 25.09 | Y | C |
| ATOM | 7646 | CE1 | TYR | 70 | 77.562 | 53.365 | 36.158 | 1.00 | 25.09 | Y | C |
| ATOM | 7647 | CD2 | TYR | 70 | 77.787 | 51.577 | 38.275 | 1.00 | 25.09 | Y | C |
| ATOM | 7648 | CE2 | TYR | 70 | 78.906 | 52.299 | 37.848 | 1.00 | 25.09 | Y | C |
| ATOM | 7649 | CZ | TYR | 70 | 78.785 | 53.194 | 36.790 | 1.00 | 25.09 | Y | C |
| ATOM | 7650 | OH | TYR | 70 | 79.873 | 53.933 | 36.382 | 1.00 | 25.09 | Y | O |
| ATOM | 7651 | C | TYR | 70 | 73.184 | 51.267 | 39.523 | 1.00 | 27.55 | Y | C |
| ATOM | 7652 | O | TYR | 70 | 72.920 | 50.545 | 40.488 | 1.00 | 27.55 | Y | O |
| ATOM | 7653 | N | THR | 71 | 72.270 | 51.635 | 38.627 | 1.00 | 38.36 | Y | N |
| ATOM | 7654 | CA | THR | 71 | 70.893 | 51.184 | 38.767 | 1.00 | 38.36 | Y | C |
| ATOM | 7655 | CB | THR | 71 | 70.074 | 52.152 | 39.657 | 1.00 | 44.65 | Y | C |
| ATOM | 7656 | OG1 | THR | 71 | 69.921 | 53.403 | 38.978 | 1.00 | 44.65 | Y | O |
| ATOM | 7657 | CG2 | THR | 71 | 70.770 | 52.394 | 40.989 | 1.00 | 44.65 | Y | C |
| ATOM | 7658 | C | THR | 71 | 70.099 | 50.991 | 37.473 | 1.00 | 38.36 | Y | C |
| ATOM | 7659 | O | THR | 71 | 70.281 | 51.707 | 36.485 | 1.00 | 38.36 | Y | O |
| ATOM | 7660 | N | LEU | 72 | 69.216 | 50.001 | 37.499 | 1.00 | 32.67 | Y | N |
| ATOM | 7661 | CA | LEU | 72 | 68.324 | 49.718 | 36.385 | 1.00 | 32.67 | Y | C |
| ATOM | 7662 | CB | LEU | 72 | 68.392 | 48.238 | 35.985 | 1.00 | 53.11 | Y | C |
| ATOM | 7663 | CG | LEU | 72 | 67.283 | 47.694 | 35.073 | 1.00 | 53.11 | Y | C |
| ATOM | 7664 | CD1 | LEU | 72 | 66.871 | 48.731 | 34.059 | 1.00 | 53.11 | Y | C |
| ATOM | 7665 | CD2 | LEU | 72 | 67.769 | 46.444 | 34.372 | 1.00 | 53.11 | Y | C |

Fig. 19: A-106

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 7666 | C | LEU | 72 | 66.958 | 50.056 | 36.972 | 1.00 | 32.67 | Y | C |
| ATOM | 7667 | O | LEU | 72 | 66.688 | 49.738 | 38.129 | 1.00 | 32.67 | Y | O |
| ATOM | 7668 | N | THR | 73 | 66.106 | 50.715 | 36.195 | 1.00 | 42.60 | Y | N |
| ATOM | 7669 | CA | THR | 73 | 64.795 | 51.100 | 36.700 | 1.00 | 42.60 | Y | C |
| ATOM | 7670 | CB | THR | 73 | 64.780 | 52.597 | 37.094 | 1.00 | 57.15 | Y | C |
| ATOM | 7671 | OG1 | THR | 73 | 66.018 | 52.943 | 37.730 | 1.00 | 57.15 | Y | O |
| ATOM | 7672 | CG2 | THR | 73 | 63.639 | 52.879 | 38.058 | 1.00 | 57.15 | Y | C |
| ATOM | 7673 | C | THR | 73 | 63.665 | 50.854 | 35.708 | 1.00 | 42.60 | Y | C |
| ATOM | 7674 | O | THR | 73 | 63.791 | 51.132 | 34.516 | 1.00 | 42.60 | Y | O |
| ATOM | 7675 | N | ILE | 74 | 62.564 | 50.316 | 36.212 | 1.00 | 51.99 | Y | N |
| ATOM | 7676 | CA | ILE | 74 | 61.396 | 50.068 | 35.386 | 1.00 | 51.99 | Y | C |
| ATOM | 7677 | CB | ILE | 74 | 60.934 | 48.597 | 35.455 | 1.00 | 52.44 | Y | C |
| ATOM | 7678 | CG2 | ILE | 74 | 60.081 | 48.271 | 34.231 | 1.00 | 52.44 | Y | C |
| ATOM | 7679 | CG1 | ILE | 74 | 62.138 | 47.656 | 35.471 | 1.00 | 52.44 | Y | C |
| ATOM | 7680 | CD1 | ILE | 74 | 61.757 | 46.182 | 35.513 | 1.00 | 52.44 | Y | C |
| ATOM | 7681 | C | ILE | 74 | 60.314 | 50.963 | 35.988 | 1.00 | 51.99 | Y | C |
| ATOM | 7682 | O | ILE | 74 | 59.739 | 50.639 | 37.030 | 1.00 | 51.99 | Y | O |
| ATOM | 7683 | N | SER | 75 | 60.058 | 52.094 | 35.335 | 1.00 | 41.67 | Y | N |
| ATOM | 7684 | CA | SER | 75 | 59.069 | 53.066 | 35.801 | 1.00 | 41.67 | Y | C |
| ATOM | 7685 | CB | SER | 75 | 59.090 | 54.291 | 34.889 | 1.00 | 51.63 | Y | C |
| ATOM | 7686 | OG | SER | 75 | 58.934 | 53.909 | 33.535 | 1.00 | 51.63 | Y | O |
| ATOM | 7687 | C | SER | 75 | 57.644 | 52.524 | 35.901 | 1.00 | 41.67 | Y | C |
| ATOM | 7688 | O | SER | 75 | 56.885 | 52.924 | 36.777 | 1.00 | 41.67 | Y | O |
| ATOM | 7689 | N | SER | 76 | 57.280 | 51.627 | 34.993 | 1.00 | 62.86 | Y | N |
| ATOM | 7690 | CA | SER | 76 | 55.950 | 51.032 | 34.996 | 1.00 | 62.86 | Y | C |
| ATOM | 7691 | CB | SER | 76 | 55.045 | 51.724 | 33.980 | 1.00 | 71.45 | Y | C |
| ATOM | 7692 | OG | SER | 76 | 53.779 | 51.086 | 33.932 | 1.00 | 71.45 | Y | O |
| ATOM | 7693 | C | SER | 76 | 56.056 | 49.558 | 34.649 | 1.00 | 62.86 | Y | C |
| ATOM | 7694 | O | SER | 76 | 55.970 | 49.176 | 33.480 | 1.00 | 62.86 | Y | O |
| ATOM | 7695 | N | LEU | 77 | 56.237 | 48.734 | 35.675 | 1.00 | 53.25 | Y | N |
| ATOM | 7696 | CA | LEU | 77 | 56.380 | 47.298 | 35.490 | 1.00 | 53.25 | Y | C |
| ATOM | 7697 | CB | LEU | 77 | 56.342 | 46.596 | 36.841 | 1.00 | 41.03 | Y | C |
| ATOM | 7698 | CG | LEU | 77 | 57.317 | 45.433 | 37.008 | 1.00 | 41.03 | Y | C |
| ATOM | 7699 | CD1 | LEU | 77 | 56.911 | 44.632 | 38.239 | 1.00 | 41.03 | Y | C |
| ATOM | 7700 | CD2 | LEU | 77 | 57.310 | 44.548 | 35.766 | 1.00 | 41.03 | Y | C |
| ATOM | 7701 | C | LEU | 77 | 55.303 | 46.703 | 34.590 | 1.00 | 53.25 | Y | C |
| ATOM | 7702 | O | LEU | 77 | 54.114 | 46.944 | 34.787 | 1.00 | 53.25 | Y | O |
| ATOM | 7703 | N | GLN | 78 | 55.723 | 45.921 | 33.602 | 1.00 | 82.27 | Y | N |
| ATOM | 7704 | CA | GLN | 78 | 54.781 | 45.285 | 32.691 | 1.00 | 82.27 | Y | C |
| ATOM | 7705 | CB | GLN | 78 | 55.094 | 45.667 | 31.243 | 1.00 | 41.92 | Y | C |
| ATOM | 7706 | CG | GLN | 78 | 54.907 | 47.148 | 30.956 | 1.00 | 41.92 | Y | C |
| ATOM | 7707 | CD | GLN | 78 | 53.508 | 47.627 | 31.288 | 1.00 | 41.92 | Y | C |
| ATOM | 7708 | OE1 | GLN | 78 | 52.520 | 47.033 | 30.852 | 1.00 | 41.92 | Y | O |
| ATOM | 7709 | NE2 | GLN | 78 | 53.416 | 48.711 | 32.056 | 1.00 | 41.92 | Y | N |
| ATOM | 7710 | C | GLN | 78 | 54.830 | 43.774 | 32.852 | 1.00 | 82.27 | Y | C |
| ATOM | 7711 | O | GLN | 78 | 55.851 | 43.213 | 33.244 | 1.00 | 82.27 | Y | O |
| ATOM | 7712 | N | PRO | 79 | 53.718 | 43.093 | 32.549 | 1.00 | 81.12 | Y | N |
| ATOM | 7713 | CD | PRO | 79 | 52.505 | 43.636 | 31.915 | 1.00 | 80.96 | Y | C |
| ATOM | 7714 | CA | PRO | 79 | 53.632 | 41.636 | 32.660 | 1.00 | 81.12 | Y | C |
| ATOM | 7715 | CB | PRO | 79 | 52.198 | 41.351 | 32.225 | 1.00 | 80.96 | Y | C |
| ATOM | 7716 | CG | PRO | 79 | 51.949 | 42.426 | 31.213 | 1.00 | 80.96 | Y | C |
| ATOM | 7717 | C | PRO | 79 | 54.663 | 40.914 | 31.792 | 1.00 | 81.12 | Y | C |
| ATOM | 7718 | O | PRO | 79 | 54.865 | 39.708 | 31.914 | 1.00 | 81.12 | Y | O |
| ATOM | 7719 | N | GLU | 80 | 55.316 | 41.670 | 30.921 | 1.00 | 44.20 | Y | N |
| ATOM | 7720 | CA | GLU | 80 | 56.316 | 41.120 | 30.021 | 1.00 | 44.20 | Y | C |
| ATOM | 7721 | CB | GLU | 80 | 56.117 | 41.729 | 28.636 | 1.00 | 102.65 | Y | C |
| ATOM | 7722 | CG | GLU | 80 | 55.853 | 43.217 | 28.678 | 1.00 | 102.65 | Y | C |
| ATOM | 7723 | CD | GLU | 80 | 55.814 | 43.833 | 27.301 | 1.00 | 102.65 | Y | C |
| ATOM | 7724 | OE1 | GLU | 80 | 56.717 | 43.528 | 26.494 | 1.00 | 102.65 | Y | O |
| ATOM | 7725 | OE2 | GLU | 80 | 54.891 | 44.629 | 27.026 | 1.00 | 102.65 | Y | O |
| ATOM | 7726 | C | GLU | 80 | 57.742 | 41.368 | 30.520 | 1.00 | 44.20 | Y | C |
| ATOM | 7727 | O | GLU | 80 | 58.672 | 40.652 | 30.145 | 1.00 | 44.20 | Y | O |
| ATOM | 7728 | N | ASP | 81 | 57.902 | 42.380 | 31.371 | 1.00 | 52.34 | Y | N |
| ATOM | 7729 | CA | ASP | 81 | 59.206 | 42.733 | 31.931 | 1.00 | 52.34 | Y | C |
| ATOM | 7730 | CB | ASP | 81 | 59.167 | 44.111 | 32.593 | 1.00 | 55.47 | Y | C |
| ATOM | 7731 | CG | ASP | 81 | 58.700 | 45.195 | 31.663 | 1.00 | 55.47 | Y | C |
| ATOM | 7732 | OD1 | ASP | 81 | 58.950 | 45.085 | 30.446 | 1.00 | 55.47 | Y | O |
| ATOM | 7733 | OD2 | ASP | 81 | 58.099 | 46.171 | 32.156 | 1.00 | 55.47 | Y | O |
| ATOM | 7734 | C | ASP | 81 | 59.641 | 41.740 | 32.991 | 1.00 | 52.34 | Y | C |
| ATOM | 7735 | O | ASP | 81 | 60.649 | 41.946 | 33.673 | 1.00 | 52.34 | Y | O |
| ATOM | 7736 | N | PHE | 82 | 58.884 | 40.664 | 33.138 | 1.00 | 63.15 | Y | N |
| ATOM | 7737 | CA | PHE | 82 | 59.207 | 39.685 | 34.158 | 1.00 | 63.15 | Y | C |
| ATOM | 7738 | CB | PHE | 82 | 57.917 | 39.041 | 34.647 | 1.00 | 168.46 | Y | C |

# Fig. 19: A-107

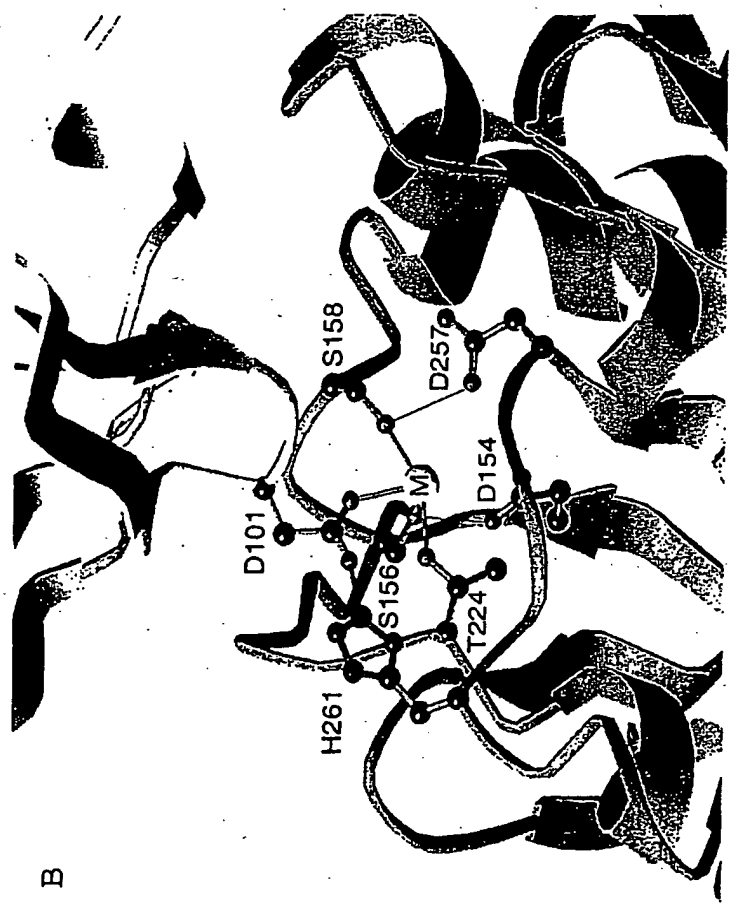
| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 7739 | CG | PHE | 82 | 57.024 | 40.004 | 35.381 | 1.00 | 168.46 | Y | C |
| ATOM | 7740 | CD1 | PHE | 82 | 57.371 | 40.454 | 36.650 | 1.00 | 168.46 | Y | C |
| ATOM | 7741 | CD2 | PHE | 82 | 55.866 | 40.498 | 34.791 | 1.00 | 168.46 | Y | C |
| ATOM | 7742 | CE1 | PHE | 82 | 56.579 | 41.384 | 37.321 | 1.00 | 168.46 | Y | C |
| ATOM | 7743 | CE2 | PHE | 82 | 55.067 | 41.430 | 35.458 | 1.00 | 168.46 | Y | C |
| ATOM | 7744 | CZ | PHE | 82 | 55.425 | 41.872 | 36.724 | 1.00 | 168.46 | Y | C |
| ATOM | 7745 | C | PHE | 82 | 60.238 | 38.657 | 33.742 | 1.00 | 63.15 | Y | C |
| ATOM | 7746 | O | PHE | 82 | 59.960 | 37.733 | 32.979 | 1.00 | 63.15 | Y | O |
| ATOM | 7747 | N | ALA | 83 | 61.447 | 38.867 | 34.256 | 1.00 | 34.42 | Y | N |
| ATOM | 7748 | CA | ALA | 83 | 62.601 | 38.015 | 34.000 | 1.00 | 34.42 | Y | C |
| ATOM | 7749 | CB | ALA | 83 | 63.138 | 38.260 | 32.595 | 1.00 | 53.93 | Y | C |
| ATOM | 7750 | C | ALA | 83 | 63.669 | 38.353 | 35.036 | 1.00 | 34.42 | Y | C |
| ATOM | 7751 | O | ALA | 83 | 63.389 | 39.033 | 36.025 | 1.00 | 34.42 | Y | O |
| ATOM | 7752 | N | THR | 84 | 64.890 | 37.877 | 34.821 | 1.00 | 50.51 | Y | N |
| ATOM | 7753 | CA | THR | 84 | 65.968 | 38.161 | 35.758 | 1.00 | 50.51 | Y | C |
| ATOM | 7754 | CB | THR | 84 | 66.566 | 36.849 | 36.323 | 1.00 | 63.35 | Y | C |
| ATOM | 7755 | OG1 | THR | 84 | 67.888 | 37.096 | 36.819 | 1.00 | 63.35 | Y | O |
| ATOM | 7756 | CG2 | THR | 84 | 66.584 | 35.766 | 35.260 | 1.00 | 63.35 | Y | C |
| ATOM | 7757 | C | THR | 84 | 67.028 | 39.021 | 35.065 | 1.00 | 50.51 | Y | C |
| ATOM | 7758 | O | THR | 84 | 67.474 | 38.708 | 33.959 | 1.00 | 50.51 | Y | O |
| ATOM | 7759 | N | TYR | 85 | 67.401 | 40.119 | 35.723 | 1.00 | 40.66 | Y | N |
| ATOM | 7760 | CA | TYR | 85 | 68.364 | 41.076 | 35.187 | 1.00 | 40.66 | Y | C |
| ATOM | 7761 | CB | TYR | 85 | 67.819 | 42.503 | 35.330 | 1.00 | 42.00 | Y | C |
| ATOM | 7762 | CG | TYR | 85 | 66.476 | 42.693 | 34.668 | 1.00 | 42.00 | Y | C |
| ATOM | 7763 | CD1 | TYR | 85 | 65.330 | 42.084 | 35.185 | 1.00 | 42.00 | Y | C |
| ATOM | 7764 | CE1 | TYR | 85 | 64.110 | 42.163 | 34.521 | 1.00 | 42.00 | Y | C |
| ATOM | 7765 | CD2 | TYR | 85 | 66.363 | 43.401 | 33.472 | 1.00 | 42.00 | Y | C |
| ATOM | 7766 | CE2 | TYR | 85 | 65.148 | 43.486 | 32.800 | 1.00 | 42.00 | Y | C |
| ATOM | 7767 | CZ | TYR | 85 | 64.028 | 42.860 | 33.327 | 1.00 | 42.00 | Y | C |
| ATOM | 7768 | OH | TYR | 85 | 62.841 | 42.889 | 32.633 | 1.00 | 42.00 | Y | O |
| ATOM | 7769 | C | TYR | 85 | 69.746 | 41.012 | 35.816 | 1.00 | 40.66 | Y | C |
| ATOM | 7770 | O | TYR | 85 | 69.891 | 40.982 | 37.042 | 1.00 | 40.66 | Y | O |
| ATOM | 7771 | N | TYR | 86 | 70.756 | 41.016 | 34.949 | 1.00 | 43.34 | Y | N |
| ATOM | 7772 | CA | TYR | 86 | 72.159 | 40.970 | 35.349 | 1.00 | 43.34 | Y | C |
| ATOM | 7773 | CB | TYR | 86 | 72.890 | 39.833 | 34.633 | 1.00 | 34.52 | Y | C |
| ATOM | 7774 | CG | TYR | 86 | 72.406 | 38.441 | 34.941 | 1.00 | 34.52 | Y | C |
| ATOM | 7775 | CD1 | TYR | 86 | 72.902 | 37.731 | 36.040 | 1.00 | 34.52 | Y | C |
| ATOM | 7776 | CE1 | TYR | 86 | 72.472 | 36.433 | 36.303 | 1.00 | 34.52 | Y | C |
| ATOM | 7777 | CD2 | TYR | 86 | 71.466 | 37.820 | 34.118 | 1.00 | 34.52 | Y | C |
| ATOM | 7778 | CE2 | TYR | 86 | 71.031 | 36.530 | 34.375 | 1.00 | 34.52 | Y | C |
| ATOM | 7779 | CZ | TYR | 86 | 71.538 | 35.841 | 35.462 | 1.00 | 34.52 | Y | C |
| ATOM | 7780 | OH | TYR | 86 | 71.124 | 34.549 | 35.683 | 1.00 | 34.52 | Y | O |
| ATOM | 7781 | C | TYR | 86 | 72.873 | 42.259 | 34.957 | 1.00 | 43.34 | Y | C |
| ATOM | 7782 | O | TYR | 86 | 72.662 | 42.780 | 33.851 | 1.00 | 43.34 | Y | O |
| ATOM | 7783 | N | CYS | 87 | 73.706 | 42.773 | 35.862 | 1.00 | 31.05 | Y | N |
| ATOM | 7784 | CA | CYS | 87 | 74.499 | 43.945 | 35.548 | 1.00 | 31.05 | Y | C |
| ATOM | 7785 | C | CYS | 87 | 75.857 | 43.346 | 35.237 | 1.00 | 31.05 | Y | C |
| ATOM | 7786 | O | CYS | 87 | 76.171 | 42.248 | 35.707 | 1.00 | 31.05 | Y | O |
| ATOM | 7787 | CB | CYS | 87 | 74.587 | 44.922 | 36.721 | 1.00 | 63.19 | Y | C |
| ATOM | 7788 | SG | CYS | 87 | 75.151 | 44.318 | 38.354 | 1.00 | 63.19 | Y | S |
| ATOM | 7789 | N | GLN | 88 | 76.653 | 44.040 | 34.431 | 1.00 | 35.54 | Y | N |
| ATOM | 7790 | CA | GLN | 88 | 77.964 | 43.536 | 34.058 | 1.00 | 35.54 | Y | C |
| ATOM | 7791 | CB | GLN | 88 | 77.834 | 42.732 | 32.769 | 1.00 | 42.46 | Y | C |
| ATOM | 7792 | CG | GLN | 88 | 79.114 | 42.125 | 32.259 | 1.00 | 42.46 | Y | C |
| ATOM | 7793 | CD | GLN | 88 | 79.594 | 42.783 | 30.983 | 1.00 | 42.46 | Y | C |
| ATOM | 7794 | OE1 | GLN | 88 | 78.834 | 42.928 | 30.019 | 1.00 | 42.46 | Y | O |
| ATOM | 7795 | NE2 | GLN | 88 | 80.863 | 43.183 | 30.965 | 1.00 | 42.46 | Y | N |
| ATOM | 7796 | C | GLN | 88 | 78.930 | 44.691 | 33.873 | 1.00 | 35.54 | Y | C |
| ATOM | 7797 | O | GLN | 88 | 78.530 | 45.774 | 33.436 | 1.00 | 35.54 | Y | O |
| ATOM | 7798 | N | GLN | 89 | 80.195 | 44.465 | 34.216 | 1.00 | 24.85 | Y | N |
| ATOM | 7799 | CA | GLN | 89 | 81.208 | 45.502 | 34.082 | 1.00 | 24.85 | Y | C |
| ATOM | 7800 | CB | GLN | 89 | 81.794 | 45.851 | 35.458 | 1.00 | 29.69 | Y | C |
| ATOM | 7801 | CG | GLN | 89 | 82.481 | 44.722 | 36.182 | 1.00 | 29.69 | Y | C |
| ATOM | 7802 | CD | GLN | 89 | 83.903 | 44.496 | 35.696 | 1.00 | 29.69 | Y | C |
| ATOM | 7803 | OE1 | GLN | 89 | 84.676 | 45.442 | 35.535 | 1.00 | 29.69 | Y | O |
| ATOM | 7804 | NE2 | GLN | 89 | 84.261 | 43.238 | 35.476 | 1.00 | 29.69 | Y | N |
| ATOM | 7805 | C | GLN | 89 | 82.294 | 45.043 | 33.128 | 1.00 | 24.85 | Y | C |
| ATOM | 7806 | O | GLN | 89 | 82.527 | 43.853 | 32.990 | 1.00 | 24.85 | Y | O |
| ATOM | 7807 | N | TRP | 90 | 82.943 | 45.993 | 32.460 | 1.00 | 39.13 | Y | N |
| ATOM | 7808 | CA | TRP | 90 | 84.008 | 45.672 | 31.510 | 1.00 | 39.13 | Y | C |
| ATOM | 7809 | CB | TRP | 90 | 83.529 | 45.955 | 30.069 | 1.00 | 30.35 | Y | C |
| ATOM | 7810 | CG | TRP | 90 | 83.422 | 47.437 | 29.678 | 1.00 | 30.35 | Y | C |
| ATOM | 7811 | CD2 | TRP | 90 | 83.088 | 47.967 | 28.385 | 1.00 | 30.35 | Y | C |

Fig. 19: A-108

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 7812 | CE2 | TRP | 90 | 83.122 | 49.375 | 28.486 | 1.00 | 30.35 | Y | C |
| ATOM | 7813 | CE3 | TRP | 90 | 82.762 | 47.389 | 27.152 | 1.00 | 30.35 | Y | C |
| ATOM | 7814 | CD1 | TRP | 90 | 83.635 | 48.523 | 30.484 | 1.00 | 30.35 | Y | C |
| ATOM | 7815 | NE1 | TRP | 90 | 83.460 | 49.686 | 29.776 | 1.00 | 30.35 | Y | N |
| ATOM | 7816 | CZ2 | TRP | 90 | 82.840 | 50.217 | 27.398 | 1.00 | 30.35 | Y | C |
| ATOM | 7817 | CZ3 | TRP | 90 | 82.480 | 48.232 | 26.063 | 1.00 | 30.35 | Y | C |
| ATOM | 7818 | CH2 | TRP | 90 | 82.522 | 49.627 | 26.199 | 1.00 | 30.35 | Y | C |
| ATOM | 7819 | C | TRP | 90 | 85.290 | 46.457 | 31.816 | 1.00 | 39.13 | Y | C |
| ATOM | 7820 | O | TRP | 90 | 86.293 | 46.339 | 31.115 | 1.00 | 39.13 | Y | O |
| ATOM | 7821 | N | SER | 91 | 85.251 | 47.254 | 32.876 | 1.00 | 18.51 | Y | N |
| ATOM | 7822 | CA | SER | 91 | 86.395 | 48.067 | 33.257 | 1.00 | 18.51 | Y | C |
| ATOM | 7823 | CB | SER | 91 | 85.948 | 49.152 | 34.237 | 1.00 | 45.24 | Y | C |
| ATOM | 7824 | OG | SER | 91 | 84.909 | 49.937 | 33.686 | 1.00 | 45.24 | Y | O |
| ATOM | 7825 | C | SER | 91 | 87.555 | 47.267 | 33.866 | 1.00 | 18.51 | Y | C |
| ATOM | 7826 | O | SER | 91 | 88.717 | 47.649 | 33.739 | 1.00 | 18.51 | Y | O |
| ATOM | 7827 | N | GLY | 92 | 87.241 | 46.166 | 34.534 | 1.00 | 40.34 | Y | N |
| ATOM | 7828 | CA | GLY | 92 | 88.282 | 45.360 | 35.146 | 1.00 | 40.34 | Y | C |
| ATOM | 7829 | C | GLY | 92 | 88.273 | 43.910 | 34.687 | 1.00 | 40.34 | Y | C |
| ATOM | 7830 | O | GLY | 92 | 87.248 | 43.386 | 34.244 | 1.00 | 40.34 | Y | O |
| ATOM | 7831 | N | ASN | 93 | 89.420 | 43.249 | 34.801 | 1.00 | 37.36 | Y | N |
| ATOM | 7832 | CA | ASN | 93 | 89.544 | 41.863 | 34.380 | 1.00 | 37.36 | Y | C |
| ATOM | 7833 | CB | ASN | 93 | 90.765 | 41.702 | 33.492 | 1.00 | 14.59 | Y | C |
| ATOM | 7834 | CG | ASN | 93 | 90.634 | 42.451 | 32.208 | 1.00 | 14.59 | Y | C |
| ATOM | 7835 | OD1 | ASN | 93 | 91.556 | 43.159 | 31.796 | 1.00 | 14.59 | Y | O |
| ATOM | 7836 | ND2 | ASN | 93 | 89.482 | 42.305 | 31.552 | 1.00 | 14.59 | Y | N |
| ATOM | 7837 | C | ASN | 93 | 89.668 | 40.944 | 35.574 | 1.00 | 37.36 | Y | C |
| ATOM | 7838 | O | ASN | 93 | 90.346 | 41.265 | 36.539 | 1.00 | 37.36 | Y | O |
| ATOM | 7839 | N | PRO | 94 | 89.005 | 39.783 | 35.525 | 1.00 | 28.71 | Y | N |
| ATOM | 7840 | CD | PRO | 94 | 88.990 | 38.808 | 36.629 | 1.00 | 9.29 | Y | C |
| ATOM | 7841 | CA | PRO | 94 | 88.167 | 39.322 | 34.412 | 1.00 | 28.71 | Y | C |
| ATOM | 7842 | CB | PRO | 94 | 87.940 | 37.858 | 34.745 | 1.00 | 9.29 | Y | C |
| ATOM | 7843 | CG | PRO | 94 | 87.823 | 37.904 | 36.251 | 1.00 | 9.29 | Y | C |
| ATOM | 7844 | C | PRO | 94 | 86.845 | 40.076 | 34.372 | 1.00 | 28.71 | Y | C |
| ATOM | 7845 | O | PRO | 94 | 86.418 | 40.640 | 35.384 | 1.00 | 28.71 | Y | O |
| ATOM | 7846 | N | TRP | 95 | 86.200 | 40.084 | 33.206 | 1.00 | 37.86 | Y | N |
| ATOM | 7847 | CA | TRP | 95 | 84.910 | 40.743 | 33.082 | 1.00 | 37.86 | Y | C |
| ATOM | 7848 | CB | TRP | 95 | 84.428 | 40.762 | 31.629 | 1.00 | 24.14 | Y | C |
| ATOM | 7849 | CG | TRP | 95 | 85.220 | 41.665 | 30.744 | 1.00 | 24.14 | Y | C |
| ATOM | 7850 | CD2 | TRP | 95 | 85.537 | 41.458 | 29.359 | 1.00 | 24.14 | Y | C |
| ATOM | 7851 | CE2 | TRP | 95 | 86.285 | 42.575 | 28.929 | 1.00 | 24.14 | Y | C |
| ATOM | 7852 | CE3 | TRP | 95 | 85.264 | 40.437 | 28.440 | 1.00 | 24.14 | Y | C |
| ATOM | 7853 | CD1 | TRP | 95 | 85.770 | 42.867 | 31.085 | 1.00 | 24.14 | Y | C |
| ATOM | 7854 | NE1 | TRP | 95 | 86.411 | 43.419 | 30.000 | 1.00 | 24.14 | Y | N |
| ATOM | 7855 | CZ2 | TRP | 95 | 86.765 | 42.697 | 27.624 | 1.00 | 24.14 | Y | C |
| ATOM | 7856 | CZ3 | TRP | 95 | 85.748 | 40.566 | 27.133 | 1.00 | 24.14 | Y | C |
| ATOM | 7857 | CH2 | TRP | 95 | 86.487 | 41.685 | 26.744 | 1.00 | 24.14 | Y | C |
| ATOM | 7858 | C | TRP | 95 | 83.959 | 39.922 | 33.941 | 1.00 | 37.86 | Y | C |
| ATOM | 7859 | O | TRP | 95 | 83.997 | 38.688 | 33.920 | 1.00 | 37.86 | Y | O |
| ATOM | 7860 | N | THR | 96 | 83.105 | 40.605 | 34.695 | 1.00 | 19.88 | Y | N |
| ATOM | 7861 | CA | THR | 96 | 82.192 | 39.913 | 35.582 | 1.00 | 19.88 | Y | C |
| ATOM | 7862 | CB | THR | 96 | 82.692 | 40.028 | 37.038 | 1.00 | 22.31 | Y | C |
| ATOM | 7863 | OG1 | THR | 96 | 82.747 | 41.408 | 37.404 | 1.00 | 22.31 | Y | O |
| ATOM | 7864 | CG2 | THR | 96 | 84.091 | 39.443 | 37.186 | 1.00 | 22.31 | Y | C |
| ATOM | 7865 | C | THR | 96 | 80.759 | 40.413 | 35.508 | 1.00 | 19.88 | Y | C |
| ATOM | 7866 | O | THR | 96 | 80.500 | 41.491 | 34.998 | 1.00 | 19.88 | Y | O |
| ATOM | 7867 | N | PHE | 97 | 79.839 | 39.596 | 36.015 | 1.00 | 20.15 | Y | N |
| ATOM | 7868 | CA | PHE | 97 | 78.420 | 39.912 | 36.073 | 1.00 | 20.15 | Y | C |
| ATOM | 7869 | CB | PHE | 97 | 77.580 | 38.827 | 35.397 | 1.00 | 25.28 | Y | C |
| ATOM | 7870 | CG | PHE | 97 | 77.890 | 38.613 | 33.946 | 1.00 | 25.28 | Y | C |
| ATOM | 7871 | CD1 | PHE | 97 | 79.062 | 37.994 | 33.554 | 1.00 | 25.28 | Y | C |
| ATOM | 7872 | CD2 | PHE | 97 | 76.979 | 38.990 | 32.969 | 1.00 | 25.28 | Y | C |
| ATOM | 7873 | CE1 | PHE | 97 | 79.322 | 37.750 | 32.204 | 1.00 | 25.28 | Y | C |
| ATOM | 7874 | CE2 | PHE | 97 | 77.234 | 38.748 | 31.611 | 1.00 | 25.28 | Y | C |
| ATOM | 7875 | CZ | PHE | 97 | 78.404 | 38.128 | 31.233 | 1.00 | 25.28 | Y | C |
| ATOM | 7876 | C | PHE | 97 | 78.054 | 39.931 | 37.557 | 1.00 | 20.15 | Y | C |
| ATOM | 7877 | O | PHE | 97 | 78.841 | 39.487 | 38.394 | 1.00 | 20.15 | Y | O |
| ATOM | 7878 | N | GLY | 98 | 76.875 | 40.460 | 37.879 | 1.00 | 30.22 | Y | N |
| ATOM | 7879 | CA | GLY | 98 | 76.412 | 40.488 | 39.256 | 1.00 | 30.22 | Y | C |
| ATOM | 7880 | C | GLY | 98 | 75.676 | 39.178 | 39.406 | 1.00 | 30.22 | Y | C |
| ATOM | 7881 | O | GLY | 98 | 75.506 | 38.478 | 38.405 | 1.00 | 30.22 | Y | O |
| ATOM | 7882 | N | GLN | 99 | 75.235 | 38.819 | 40.608 | 1.00 | 24.51 | Y | N |
| ATOM | 7883 | CA | GLN | 99 | 74.537 | 37.541 | 40.755 | 1.00 | 24.51 | Y | C |
| ATOM | 7884 | CB | GLN | 99 | 74.350 | 37.163 | 42.231 | 1.00 | 60.71 | Y | C |

Fig. 19: A-109

```
ATOM   7885  CG  GLN    99      74.599  38.274  43.209  1.00  60.71      Y    C
ATOM   7886  CD  GLN    99      73.728  39.464  42.945  1.00  60.71      Y    C
ATOM   7887  OE1 GLN    99      72.510  39.411  43.113  1.00  60.71      Y    O
ATOM   7888  NE2 GLN    99      74.346  40.551  42.515  1.00  60.71      Y    N
ATOM   7889  C   GLN    99      73.189  37.507  40.043  1.00  24.51      Y    C
ATOM   7890  O   GLN    99      72.587  36.443  39.894  1.00  24.51      Y    O
ATOM   7891  N   GLY   100      72.730  38.666  39.586  1.00  42.40      Y    N
ATOM   7892  CA  GLY   100      71.455  38.725  38.900  1.00  42.40      Y    C
ATOM   7893  C   GLY   100      70.355  39.043  39.886  1.00  42.40      Y    C
ATOM   7894  O   GLY   100      70.483  38.749  41.074  1.00  42.40      Y    O
ATOM   7895  N   THR   101      69.283  39.662  39.399  1.00  27.30      Y    N
ATOM   7896  CA  THR   101      68.144  40.021  40.236  1.00  27.30      Y    C
ATOM   7897  CB  THR   101      68.024  41.538  40.401  1.00  28.79      Y    C
ATOM   7898  OG1 THR   101      69.008  41.995  41.336  1.00  28.79      Y    O
ATOM   7899  CG2 THR   101      66.646  41.907  40.892  1.00  28.79      Y    C
ATOM   7900  C   THR   101      66.903  39.492  39.551  1.00  27.30      Y    C
ATOM   7901  O   THR   101      66.619  39.845  38.408  1.00  27.30      Y    O
ATOM   7902  N   LYS   102      66.166  38.635  40.240  1.00  67.88      Y    N
ATOM   7903  CA  LYS   102      64.978  38.064  39.642  1.00  67.88      Y    C
ATOM   7904  CB  LYS   102      64.806  36.618  40.106  1.00 117.75      Y    C
ATOM   7905  CG  LYS   102      63.920  35.785  39.198  1.00 117.75      Y    C
ATOM   7906  CD  LYS   102      63.925  34.321  39.608  1.00 117.75      Y    C
ATOM   7907  CE  LYS   102      63.094  33.485  38.651  1.00 117.75      Y    C
ATOM   7908  NZ  LYS   102      63.586  33.621  37.250  1.00 117.75      Y    N
ATOM   7909  C   LYS   102      63.749  38.885  39.996  1.00  67.88      Y    C
ATOM   7910  O   LYS   102      63.560  39.262  41.155  1.00  67.88      Y    O
ATOM   7911  N   VAL   103      62.926  39.176  38.989  1.00  55.50      Y    N
ATOM   7912  CA  VAL   103      61.706  39.941  39.208  1.00  55.50      Y    C
ATOM   7913  CB  VAL   103      61.779  41.349  38.510  1.00  68.46      Y    C
ATOM   7914  CG1 VAL   103      63.207  41.865  38.530  1.00  68.46      Y    C
ATOM   7915  CG2 VAL   103      61.258  41.290  37.084  1.00  68.46      Y    C
ATOM   7916  C   VAL   103      60.489  39.141  38.709  1.00  55.50      Y    C
ATOM   7917  O   VAL   103      60.378  38.828  37.517  1.00  55.50      Y    O
ATOM   7918  N   GLU   104      59.597  38.779  39.633  1.00  70.95      Y    N
ATOM   7919  CA  GLU   104      58.395  38.025  39.281  1.00  70.95      Y    C
ATOM   7920  CB  GLU   104      58.243  36.764  40.145  1.00 145.77      Y    C
ATOM   7921  CG  GLU   104      57.957  37.019  41.616  1.00 145.77      Y    C
ATOM   7922  CD  GLU   104      59.215  37.263  42.418  1.00 145.77      Y    C
ATOM   7923  OE1 GLU   104      59.106  37.542  43.631  1.00 145.77      Y    O
ATOM   7924  OE2 GLU   104      60.315  37.167  41.839  1.00 145.77      Y    O
ATOM   7925  C   GLU   104      57.157  38.897  39.443  1.00  70.95      Y    C
ATOM   7926  O   GLU   104      57.197  39.939  40.108  1.00  70.95      Y    O
ATOM   7927  N   ILE   105      56.058  38.459  38.834  1.00 139.77      Y    N
ATOM   7928  CA  ILE   105      54.791  39.184  38.876  1.00 139.77      Y    C
ATOM   7929  CB  ILE   105      53.838  38.730  37.757  1.00 105.35      Y    C
ATOM   7930  CG2 ILE   105      52.923  39.875  37.373  1.00 105.35      Y    C
ATOM   7931  CG1 ILE   105      54.633  38.232  36.553  1.00 105.35      Y    C
ATOM   7932  CD1 ILE   105      53.775  37.746  35.397  1.00 105.35      Y    C
ATOM   7933  C   ILE   105      54.047  38.952  40.180  1.00 139.77      Y    C
ATOM   7934  O   ILE   105      53.763  37.810  40.533  1.00 139.77      Y    O
ATOM   7935  N   LYS   106      53.706  40.031  40.880  1.00 101.75      Y    N
ATOM   7936  CA  LYS   106      52.969  39.916  42.135  1.00 101.75      Y    C
ATOM   7937  CB  LYS   106      53.545  40.870  43.189  1.00  95.13      Y    C
ATOM   7938  CG  LYS   106      52.954  40.690  44.584  1.00  95.13      Y    C
ATOM   7939  CD  LYS   106      53.556  41.665  45.586  1.00  95.13      Y    C
ATOM   7940  CE  LYS   106      52.939  41.482  46.965  1.00  95.13      Y    C
ATOM   7941  NZ  LYS   106      53.446  42.478  47.948  1.00  95.13      Y    N
ATOM   7942  C   LYS   106      51.492  40.235  41.897  1.00 101.75      Y    C
ATOM   7943  O   LYS   106      51.148  40.637  40.765  1.00 100.80      Y    O
ATOM   7944  OXT LYS   106      50.694  40.080  42.844  1.00  94.18      Y    O
ATOM   7945 MN   MN    400      89.864  50.249  22.621  1.00  34.24      N
END
```



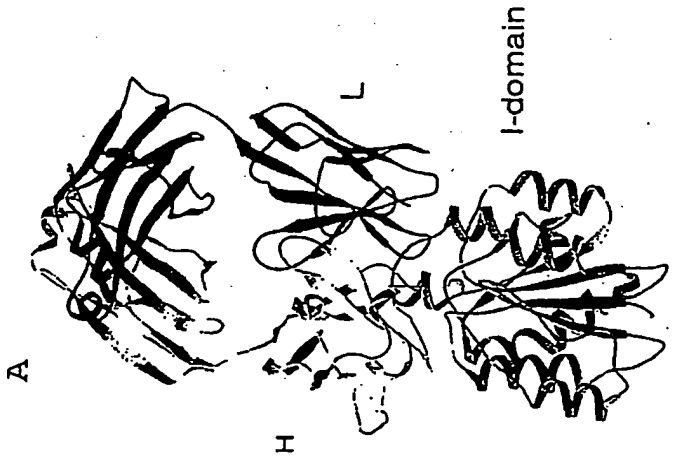




Fig. 20

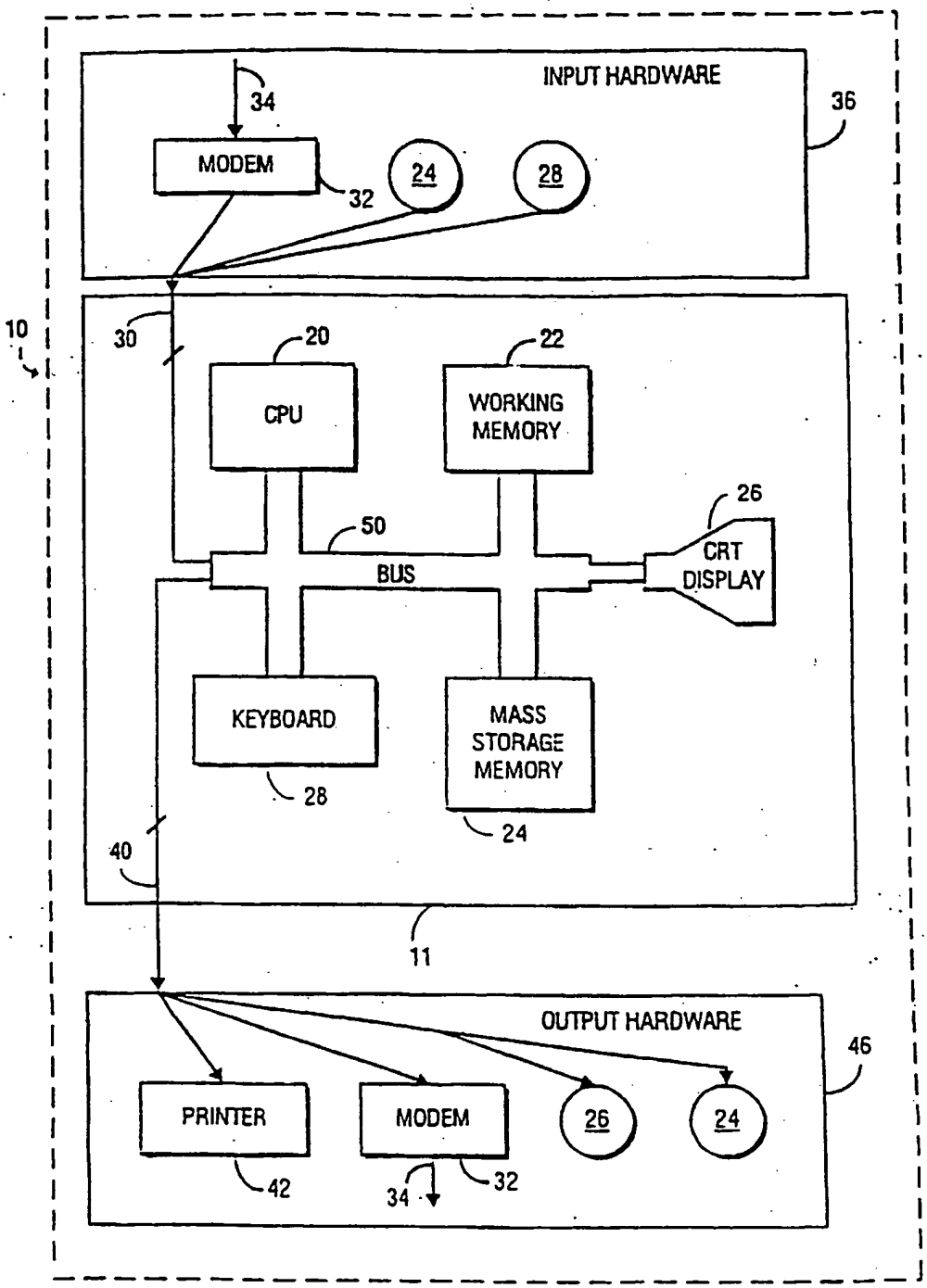

INPUT HARDWARE
36
34
MODEM
32
24
28
10
30
20
CPU
22
WORKING MEMORY
26
50
BUS
CRT DISPLAY
KEYBOARD
28
MASS STORAGE MEMORY
24
40
11
OUTPUT HARDWARE
46
PRINTER
42
MODEM
34
32
26
24

Fig. 21

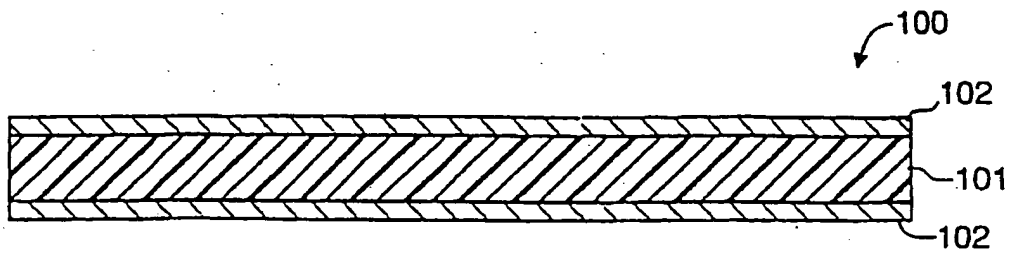



Fig. 22

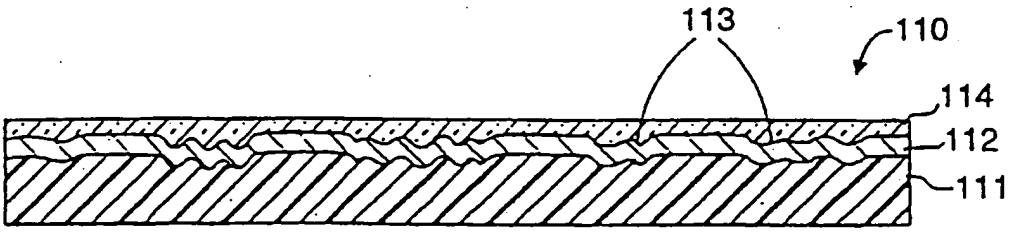



Fig. 23